Yet another thermodynamic environment

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Abstract

In a few lines, the Oldroyd-B, FENE-P, Giesekus and FENE-CR models are shown as satisfying the second principle of thermodynamics. In addition, entropy estimates (*a priori* bounds) are easily obtained, together with explicit expressions for the dissipation. For the Giesekus and FENE-CR models, these estimates are new, while for the Oldroyd-B and FENE-P, there were already established. In all cases, they are obtained here in a clear an concise manner, instead of long derivations. This approach could also be applied to the development of new constitutive equations, and some preliminary explorations are provided. The conformation tensor is identified in a purely kinematic context, in terms of the Cauchy-Green tensor. Consequently, the formulation in terms of the logarithm of conformation tensor is reinterpreted in terms of Hencky strain and its logarithmic corotational derivative. While useful for numerical computations, this also leads to much more concise and understandable formulations, but above all, it opens up new avenues for theoretical developments. This paper presents new developments of a work initiated by the author in a recent book (Springer, 2024), which is also reviewed here in a concise manner. We briefly recall how the standard generalized materials framework extends to large-strains kinematics in Eulerian frame.

Keywords: entropy estimate, second principle of thermodynamics, Hencky strain, logarithmic corotational derivative, viscoelastic fluids, standard generalized materials,

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1. Introduction

Figure 1: A bouncing ball captured with a stroboscopic flash at 25 images per second. Michael Maggs, 2007 (adapted ; license: CC-BY-SA-3.0).

What is thermodynamics ?

Observe on Fig. 1 the bouncing ball. As the ball falls freely under the influence of gravity, it accelerates downward, its initial gravity potential energy converting into kinetic energy. On impact with a hard surface the ball deforms, converting the kinetic energy into elastic potential energy. As the ball springs back, the elastic energy converts back firstly to kinetic energy and then as the ball regains height into gravity potential energy. Due to inelastic-strains and air resistance, each successive bounce is lower than the last: the ball loses some of its energy.

Where did that energy go ?

The answers is given by thermodynamics: it is *dissipated*, for instance it is transformed into heat and sound. This energy is irreversibly lost for the ball, which will cease to move in a finite amount of time. So, thermodynamics has a physical meaning: it explains complex phenomena in an elegant and comprehensive manner.

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Problematic. All along this paper, potential and elastic energies are grouped into the *free energy* concept, denoted by ψ, while the *dissipation* is denoted as $\mathscr{D}$. Dissipation is always non-negative i.e. $\mathscr{D} \geqslant 0$: this expresses the irreversibility of energy loss. This inequality is a consequence of the **second principle of thermodynamics**. Mathematical models are described by two groups of equations: equations of conservation and **constitutive equations**. While equations of conservation are universals for all materials, constitutive equations are specific to some materials.

We might imagine that the variety of constitutive equations are limited only by the imagination of model designers, but this is not the case. During the development of new constitutive equations, satisfying $\mathscr{D} \geqslant 0$ appears as a constraint that strongly restricts the possibilities. Moreover, this constraint remains difficult to check in general, even for very common constitutive equations. The temptation to bypass this check during the development of new models is real and could have disastrous consequences, e.g. the unexpected divergence of simulation codes due to ill-posed problems. Imagine a mathematical model or a code predicting the ball in Fig. 1 bouncing higher and higher… So, satisfying the thermodynamic constraint $\mathscr{D} \geqslant 0$ is both difficult but of major importance for model development: it is necessary to avoid unphysical model predictions.

Context. In the past, several thermodynamic environments have been proposed to assist model designers: let's review them. The situation between solid and fluid mechanics is very contrasted.

- **Solid mechanics**. Thermodynamics of irreversible processes started in 1940 with Eckart [19] who studied viscous materials with heat conduction, see also de Groot and Mazur [16] or Šilhavý [66] for more historical references. The concept of **dissipation potential** was next introduced independently at least in 1968 by Ziegler [73], in 1972 by Verhás [71], in 1973 by Edelen [20], and in 1974 by Moreau [48]. The dissipation potential, denoted by ϕ, is such that

$$\mathscr{D} = \dot{\boldsymbol{\alpha}}.\nabla\phi(\dot{\boldsymbol{\alpha}}) \geqslant 0 \tag{1}$$

where $\boldsymbol{\alpha}$ denotes the set of thermodynamic states and $\dot{\boldsymbol{\alpha}}$, the corresponding rates. The dissipation potential extends to the nonlinear case the Onsager [51] linear reciprocal relations, which corresponds the quadratic choice $\phi(\dot{\boldsymbol{\alpha}}) = \dot{\boldsymbol{\alpha}}^T M \dot{\boldsymbol{\alpha}}/2$, and where M is the Onsager symmetric non-negative matrix. In 1975, Halphen and Nguyen [31] proposed the environment of *generalized standard materials*, that is based on this possibly non-smooth dissipation potential ϕ. This clear and efficient environment is still widely used in solid mechanics, see e.g. Maugin [47] for applications. Extensions from small to large-strains have been then considered in a Lagrangian frame, see e.g. Sidoroff and Dogui [65]. Nevertheless, such extensions focused on some specific applications, e.g. elastoplasticity, and there are no general environment available yet. Moreover, if the Lagrangian frame is applicable in solid mechanics, where strains are bounded, it has severe limitations in fluid mechanics, where strains are generally unbounded. A long time process would develop huge strains and stationary solutions are not reachable in this way. In that case, an Eulerian frame is preferred.

- **Fluid mechanics**. For complex fluids and soft solids in large-strains, possibly unbounded, different approaches were developed. In 1964, Kluitenberg [40] extended the Kelvin-Voigt viscoelastic solid model to incorporate large-strains and proposed for the first time large-strains kinematics in both Lagrangian and Eulerian frames. Next, in 1976, Leonov [42] extended this work to viscoelastic fluids in large-strains with an Eulerian frame. In 1984, Grmela [27] proposed the Poisson bracket as an abstract thermodynamic formalism for model development. In 1988, Ait-Kadi et al. [1, eqn (19)] (see also Grmela [28]) proposed for the first time the correct expressions for the free energy ψ of both the Oldroyd-B and FENE-P models. Nevertheless, these authors neither addressed the second principle nor computed the dissipation $\mathscr{D}$. In 1990, Beris and Edwards [5] (see also [6]) proposed new developments of the Poisson bracket formalism and analyzed most common viscoelastic fluid models: for each model, the second principle of thermodynamics was for the fist time successfully checked via the non-negativity of the Onsager matrix (see their eqn (4.1), p. 525). Next, in 1992, Leonov [43] systematically studied most common viscoelastic fluid models and proposed some expressions for both the free energy ψ and the dissipation $\mathscr{D}$. But surprisingly, while his computations were correct throughout his article, its final results are incorrect for both the Oldroyd-B and FENE-P models and for the two expressions of ψ and $\mathscr{D}$, see his eqns (52) and (55). Thus, unfortunately, despite his solid and important theoretical work, this author was not able to conclude that these models satisfy the second principle. Note that these incorrect expressions of $\mathscr{D}$ were then reused later without verification, see e.g. Pasquali and Scriven [53, p. 125, table 2]. In 1997, Grmela and Öttinger [29] extended the Poisson bracket formalism as the GENERIC one (see also [52]). In 1999, with the help of this formalism, Dressler et al. [18] studied some non-isothermal viscoelastic fluids models and checked the second principle of thermodynamics via the non-negativity of the Onsager matrix. In 2008, Hütter and Tervoort [36], also using the GENERIC formalism, studied both anisotropic and non-isothermal viscoelasticity. See Beris [4] for a recent review of these formalisms.

Entropy estimate. Variational methods for proving the existence of a coupled system of partial differential equations emerged in 1934 with the pioneering work of Leray [44] on the Navier-Stokes equations (see also Temam [70, p. 189]). The first step is to prove some *a priori* bounds verified by any possible solution. Thanks to these bounds, the second step is to show that the limit of a bounded sequence of finite-dimensional approximations of this solution converges, thus proving the existence of the solution as this limit. Let us briefly review the mathematical work developed to prove the existence of solutions of complex fluid flow problems. The Oldroyd-B model [49] was proposed in 1950. In 1985, Renardy [57] proved the existence of stationary solutions. Then, in 1990, Guillopé and Saut [30] proved the existence of time-dependent solutions until a given time, that depends upon data (local-in-time). Only for enought small data, a solution is proved to exist at any time (global-in-time). This is a very restrictive assumption and then, many authors tried to improve this result: the challenge is to improve the*a priori* bounds. In 2000, Lions and Masmoudi [45] showed a global-in-time existence result, but for the corotational derivative, not the upper-convected one used by the Oldroyd-B model. In 2007, Hu and Lelièvre [34, p. 914] established an **entropy estimate** that provides new *a priori* bounds for both the Oldroyd-B and the FENE-P models. Based on this publication, new efficient existence results appeared soon. In 2011, using this entropy estimate, Masmoudi [46], obtained for the first time a global-in-time **existence result** for the FENE-P model. But not for the Oldroyd-B one. In 2012, Constantin and Kliegl [15] obtained a global-in-time for the Oldroyd-B model, but with an additional stress-diffusion term in the differential constitutive equation. In 2024, similarly to Hu and Lelièvre [34], for a special case of the Giesekus model, Bulíček et al. [10] established an entropy estimate and proved a global-in-time existence result. See Renardy and Thomases [58] for a recent review on existence results for the Oldroyd-B and related models.

It should be pointed out that the entropy estimate published by Hu and Lelièvre [34, p. 914] for both the Oldroyd-B and FENE-P models played a crucial role in the progress of existence results. Indeed, all the previous works on existence of solutions did not use the correct definition of the free energy for the Oldroyd-B model: these previous existence results were correct, but with too strong assumptions (e.g. small data) and thus, obtained weaker existence results. According to the addendum p. 915 in Hu and Lelièvre [34], it appears that these authors obtained independently the correct expressions of both the free energy ψ and the dissipation $\mathscr{D}$, without the aid of any previous thermodynamic publications from the complex fluid community. Thus, these authors have accomplished a difficult task, and the work is impressive.

Summary. Finally, while in solid mechanics, model design is widely based on thermodynamics, this approach is rarely adopted in fluid mechanics. Indeed, the formalism used in solid mechanics is clear but often limited, whereas in fluid mechanics, the opposite is true. The objective of this article is to fill this gap. In mathematics, the community would be also well advised to familiarize itself with thermodynamics, since the experience has shown that entropy estimates lead to very efficient *a priori* bounds that are required to prove the existence of solutions. The difficulty could be found by examining the application of the proposed thermodynamic formalisms for these complex fluids: while the formalisms are quite general and powerful, the computations are far from easy. Moreover, the formalism itself could distract both model designers and mathematicians.

Goal. Our goal is to disseminate thermodynamics in fluid mechanics: the proposed environment, called YATE, allows the clear and easy development of new constitutive equations that automatically satisfy $\mathscr{D} \geqslant 0$. Instead of writing directly constitutive relations, model designers are encouraged to first specify the free energy ψ and the dissipation potential ϕ. Then constitutive equations are automatically obtained by simple derivation of these quantities. In addition, both an explicit expression of $\mathscr{D}$ and an entropy estimate (*a priori* bounds) are also directly obtained. In order to gauge the progress represented by the YATE environment, let us remember that it took 40 years to prove that the Oldroyd-B model verified the second principle, and a further 21 years to obtain the entropy estimate.

Outline of the paper. Section 2 introduces some notations and provides global energy and entropy estimates. Next, section 3 presents an overview of standard generalized materials (SGM) in small-strains with some examples in solid and fluid mechanics, pointing out its advantages and limitations. Then, section 4 starts by extending standard generalized materials to large-strains in an Eulerian frame (YATE). To this end, we provide here a concise review of a recent book [63] by the author, in which Eulerian kinematics was reexamined and clarified. Next, we turn to examples and show in a clear and concise way that both the Oldroyd-B, FENE-P, Giesekus and FENE-CR models satisfy the second principle of thermodynamics and provide the corresponding entropy estimate. While these estimates was already known for the Oldroyd-B and FENE-P models, there are new for those of Giesekus and FENE-CR. In all cases, they are obtained here in just a few lines, instead of long derivations as was previously the case. Finally, section 5 presents a general discussion and a preliminary exploration for applying this approach during the development of new models. This paper contains two appendices. Appendix Appendix A develops the proof the estimates (theorem 1 and corollary 2) while appendix Appendix B furnishes the correspondence between the Poisson bracket formalism and present notations, together with the practical method to obtain an explicit computation of the dissipation $\mathscr{D}$ from [5, 6].

2. Notation and global estimates

2.1. Notations

	description
$\mathscr{D}$	dissipation
ϕ	dissipation potential
ψ	free energy
$\boldsymbol{v}$	velocity
$\nabla\boldsymbol{v}$	$= (\partial v_i/\partial x_j)_{i,j}$, velocity gradient
$\boldsymbol{\sigma}$	Cauchy stress
$\boldsymbol{B}$	left Cauchy-Green tensor
$\boldsymbol{B}_e$	reversible left Cauchy-Green tensor alias: *conformation tensor*
$\boldsymbol{h}$	$= (1/2)\mathbf{log}\,\boldsymbol{B}$: left Hencky strain
$\boldsymbol{h}_e$	$= (1/2)\mathbf{log}\,\boldsymbol{B}_e$ reversible left Hencky strain alias: *logarithm of conformation tensor*
$\boldsymbol{h}_p$	$= \boldsymbol{h} - \boldsymbol{h}_e$
$\boldsymbol{D}$	$= (\nabla\boldsymbol{v} + \nabla\boldsymbol{v}^T)/2$: stretching alias: *strain rate*
$\boldsymbol{D}_e$	reversible stretching
$\boldsymbol{D}_p$	$= \boldsymbol{D} - \boldsymbol{D}_e$
$\overset{\triangledown}{\boldsymbol{a}}$	upper-convected derivative
$\overset{\circ}{\boldsymbol{a}}^{(\log)}$	logarithmic corotational derivative

Table 1: Notations.

The notations used all along this paper are summarized in Table 1. The mass, momentum, and energy conservations, together with the second principle of thermodynamics, write as:

$$\dot{\rho} + \rho\,\mathrm{div}\,\boldsymbol{v} = 0 \tag{2a}$$

$$\rho\dot{\boldsymbol{v}} - \mathbf{div}\,\boldsymbol{\sigma} = \boldsymbol{f} \tag{2b}$$

$$\rho\dot{e} + \mathrm{div}\,\boldsymbol{q} = r + \boldsymbol{\sigma}:\boldsymbol{D} \tag{2c}$$

$$\rho\dot{s} + \mathrm{div}\left(\frac{\boldsymbol{q}}{\theta}\right) - \frac{r}{\theta} = \frac{\mathscr{D}}{\theta} \geqslant 0 \tag{2d}$$

Here, ρ is the mass density, $\boldsymbol{v}$, the velocity and $\boldsymbol{\sigma}$, the symmetric Cauchy stress tensor. As usual, the dot on the top of a quantity denotes its Lagrangian derivative, e.g. $\dot{\rho} = \partial_t\rho + (\boldsymbol{v}.\nabla)\rho$, also called convective or material derivative. Also, $\boldsymbol{f}$ denotes the external forces, e.g. the gravity forces. Next, e is the internal energy, s, the entropy, $\theta > 0$, the temperature and $\boldsymbol{q}$, the heat flux, while r is the heat sources. The dissipation $\mathscr{D}$ is defined from (2d). By definition, the internal energy e and free energy ψ are functions: e is convex versus s and ψ is concave versus θ, while both functions optionally depend upon others thermodynamic state variables, usually the strain and some others internal state variables. We also assume that both e and ψ are bounded from below versus all these others optional state variables, and, without loss of generality, we could assume $e \geqslant 0$ and $\psi \geqslant 0$. They are linked together via a Legendre transform with the optimality relations:

$$e(s) = \psi(\theta) + s\theta, \;\; s = -\frac{\partial_\psi}{\partial \theta}(\theta) \text{ and } \theta = \frac{\partial e}{\partial s}(s) \qquad (2e)$$

So, in order to describe a specific material, only one of these two functions, either e or ψ, should be specified. Assume for instance that our material is specified via $\psi(\theta)$. Then $s = -\partial_\theta \psi(\theta)$ and $e = \psi(\theta) + s\,\theta$ are deduced as expressions of θ. Conversely, our material could be specified equivalently via $e(s)$.

Summary. Assume that $\psi(\theta)$ and the right-hand-sides $\boldsymbol{f}$ and r are known, it remains five unknowns $(\rho, \boldsymbol{v}, \theta, \boldsymbol{\sigma}, \boldsymbol{q})$ for only three conservation equations (2a)-(2c) and the constraint (2d). The usual approach in order to close the system of equations is to provide some additional **constitutive equations** for $\boldsymbol{\sigma}$, and $\boldsymbol{q}$ versus $(\rho, \boldsymbol{v}, \theta)$. For an isothermal process, assuming that the free energy ψ is known versus optional thermodynamic states, it remains three unknowns $(\rho, \boldsymbol{v}, \boldsymbol{\sigma})$ for only two conservation equations (2a)-(2b) and the constraint (2d). We have to provide additional constitutive equations for $\boldsymbol{\sigma}$ versus $(\rho, \boldsymbol{v})$. For instance, the Newtonian model $\boldsymbol{\sigma} = 2\eta_0 \boldsymbol{D}$ with $\psi = 0$ closes the system of equations, where $\eta_0 \geqslant 0$ is the viscosity and $\boldsymbol{D} = (\nabla \boldsymbol{v} + \nabla \boldsymbol{v})/2$ denotes the stretching, also called strain rate. In that case, the dissipation writes simply $\mathscr{D} = \boldsymbol{\sigma} : \boldsymbol{D} = 2\eta_0 |\boldsymbol{D}|^2 \geqslant 0$.

2.2. *Global estimates*

Let us consider a thermodynamic system described by (2a)-(2e).

Definition 1 (isolated system)**.**
Let $\Omega \subset \mathbb{R}^N$ be the flow domain, where $N \geqslant 1$ is the physical space dimension, e.g. $N = 3$.

A system is said isolated when

1. the right-hand-sides $\boldsymbol{f}$ and r in (2b)-(2c) are zero.
2. and either $\partial\Omega = \varnothing$ (e.g. periodic boundary conditions, or $\Omega = \mathbb{R}^N$ the whole universe) or the two boundary fluxes $\boldsymbol{\sigma n}$ and $\boldsymbol{q.n}$ are zero, where $\boldsymbol{n}$ denotes the unit outward normal on $\partial\Omega$.

Theorem 1 (global estimates)**.**
Assume that the system is isolated. Then, the global energy, i.e. the global sum of the kinetic and internal energies, is conserved, while its global entropy is growing:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \rho \left(\frac{|\boldsymbol{v}|^2}{2} + e \right) = 0 \qquad (3a)$$

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \rho s = \int_\Omega \frac{\mathscr{D}}{\theta} \geqslant 0 \qquad (3b)$$

Proof: See appendix Appendix A. ■

Corollary 2 (isothermal global entropy estimate)**.**

Assume that the system is isolated and isotherm (θ is constant). Then the following estimate holds:

$$\frac{\mathrm{d}}{\mathrm{d}t} \int_\Omega \rho \left(\frac{|\boldsymbol{v}|^2}{2} + \psi \right) + \int_\Omega \mathscr{D} = 0 \qquad (4)$$

Proof: See appendix Appendix A. ■

Note that, in (4), the time derivative applies to the global sum of the kinetic and free energies. Since $\mathscr{D} \geqslant 0$, then this global sum is decreasing and uniformly bounded from above by its initial value:

$$\int_\Omega \rho \left(\frac{|\boldsymbol{v}|^2}{2} + \psi \right) + \int_0^t\!\!\int_\Omega \mathscr{D} = \int_\Omega \rho \left(\frac{|\boldsymbol{v}|^2}{2} + \psi \right)_{|t=0}$$

Since $\psi \geqslant 0$, this estimate proves that both the global kinetic energy $\int_\Omega \rho|\boldsymbol{v}|^2/2$, the global free energy $\int_\Omega \rho\psi$ and also the cumulated global dissipation $\int_0^t \int_\Omega \mathscr{D}$ remain uniformly bounded, at any time t. Finally, this entropy estimate yields some *a priori* bounds on $\boldsymbol{v}$ and on the thermodynamic state variables involved in the expressions of ψ and $\mathscr{D}$. These bounds constitute the starting point for proving of existence of solutions of the system of partial differential equations.

3. Standard generalized materials

This section starts by defining standard generalized materials, as introduced in 1975 by Halphen and Nguyen [31] with the small-strains assumption. For simplicity, we focuses on isothermal processes, i.e. θ is constant. Next, we turn to examples, pointing out the clarity and efficiency of this environment. A discussion on its limitations closes this section.

3.1. Definition

A standard generalized material (SGM) is completely defined by two functions: the free energy ψ and the dissipation potential ϕ. The free energy ψ is assumed to depend upon the set of m thermodynamic *states* denoted by $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_m)$, $m \geqslant 1$ and the dependency of the function ψ upon the states variables $\boldsymbol{\alpha}$ is denoted as $\psi(\boldsymbol{\alpha})$. By convention $\alpha_1 = \boldsymbol{\varepsilon}$ is the linearised strain tensor. When $m \geqslant 2$, then $(\alpha_i)_{2\leqslant i\leqslant m}$ represents $m-1$ thermodynamic *internal state variables.* Let $\dot{\boldsymbol{\alpha}} = (\dot{\alpha}_1, \dot{\alpha}_2, \ldots, \dot{\alpha}_m)$ be the set of Lagrangian derivatives of the thermodynamic states, called the thermodynamic *rates of states.* Then $\dot{\alpha}_1 = \dot{\boldsymbol{\varepsilon}} = \boldsymbol{D} = (\nabla\boldsymbol{v} + \nabla\boldsymbol{v}^T)/2$ is the strain rate tensor. The dissipation potential ϕ is assumed to depend upon the rates of states $\dot{\boldsymbol{\alpha}}$, and the dependency of the function ϕ upon the rates variables $\dot{\boldsymbol{\alpha}}$ is denoted as $\phi(\dot{\boldsymbol{\alpha}})$. Optionally, ϕ could also depend upon the states $\boldsymbol{\alpha}$ as parameters, and in that case, it will be denoted as $\phi([\boldsymbol{\alpha}];\ \dot{\boldsymbol{\alpha}})$.

Then, the constitutive equations of the material are given by

$$\begin{cases} \boldsymbol{\sigma} = \rho\dfrac{\partial\psi}{\partial\boldsymbol{\varepsilon}}(\boldsymbol{\alpha}) + \dfrac{\partial\phi}{\partial\dot{\boldsymbol{\varepsilon}}}(\dot{\boldsymbol{\alpha}}), & (i=1) \qquad \text{(5a)} \\ 0 = \rho\dfrac{\partial\psi}{\partial\alpha_i}(\boldsymbol{\alpha}) + \dfrac{\partial\phi}{\partial\dot{\alpha}_i}(\dot{\boldsymbol{\alpha}}), & 2\leqslant i\leqslant m \qquad \text{(5b)} \end{cases}$$

This definition extends to the case where the dissipation potential ϕ is not differentiable, e.g. for materials involving plasticity, friction or damage. When ϕ is convex, $\partial\phi/\partial\dot{\alpha}_i$ denotes the subdifferential of ϕ with respect to $\dot{\boldsymbol{\alpha}}_i$, see e.g. [61, p. 94]. Otherwise, when ϕ is neither differentiable nor convex, assuming only Lipschitzian regularity, then, it admits a Clarke [13, p. 10] derivative and the notation $\partial\phi/\partial\dot{\alpha}_i$ interprets as the convex hull of all directional derivatives. In these cases, the previous constitutive equations are simply adjusted by replacing the equal "=" symbol by the belongs to "∈" one.

A major difficulty for constitutive equations is to check that the second principle of thermodynamics is satisfied. A definitive advantage of the generalized standard materials is the possibility to have a sufficient condition on the dissipation of energy for the second principle to be satisfied, and that this condition is easy to check. The following result presents this property.

Theorem 2 (second principles, small-strains)**.** Assume that the dissipation potential ϕ is nonnegative ($\phi \geqslant 0$), convex at $\dot{\boldsymbol{\alpha}} = 0$ and vanish in zero, i.e. $\phi(\dot{\boldsymbol{\alpha}}=0) = 0$. Then the material described by the two functions ψ and ϕ satisfies the second principle of thermodynamics and the dissipation $\mathscr{D} \geqslant 0$ is given by (1).

Proof: see [61, p. 223]. ∎

Note that the convexity of ϕ is required only at $\dot{\boldsymbol{\alpha}} = 0$. Of course, when ϕ is convex everywhere, which is the case for most applications, e.g. when ϕ is quadratic positive, this condition is trivially satisfied. Let us turn to observe this environment in action by reviewing some classical models.

3.2. Examples

3.2.1. Hookean elastic solid

Let $m = 1$ and $\boldsymbol{\alpha} = \boldsymbol{\varepsilon}$. The Hookean elastic solid is described by

$$\begin{cases} \psi(\boldsymbol{\varepsilon}) = \dfrac{G}{\rho_0}|\boldsymbol{\varepsilon}|^2 + \dfrac{\lambda}{\rho_0}(\mathrm{tr}\,\boldsymbol{\varepsilon})^2 \\ \phi(\dot{\boldsymbol{\varepsilon}}) = 0 \end{cases}$$

and is represented on Fig. 2.top-left. Here, $\rho_0 > 0$ denotes the mass density of the material when in the rest state i.e. when $\boldsymbol{\varepsilon} = 0$. The free energy ψ collects the spring element associated to the shear and bulk elastic moduli $G > 0$ and $\lambda > -G$, and since there is no dissipative element on the diagram, the dissipation potential ϕ is zero. The zero dissipation potential ϕ satisfies the assumptions of theorem 2 and then this material satisfies the second principle of thermodynamics with $\mathscr{D} = 0$. Since $\dot{\boldsymbol{\varepsilon}} = \boldsymbol{D}$, then, from the mass conservation (2a), we have $\dot{\rho}/\rho = -\mathrm{div}\,\boldsymbol{v} = -\mathrm{tr}\,\boldsymbol{D} = -\mathrm{tr}\,\dot{\boldsymbol{\varepsilon}}$. Next, by integration, we get $\log(\rho/\rho_0) = -\mathrm{tr}\,\boldsymbol{\varepsilon}$ i.e. $\rho = \rho_0\exp(-\mathrm{tr}\,\boldsymbol{\varepsilon})$. The constitutive equation is obtained from (5a):

$$\begin{aligned} \boldsymbol{\sigma} &= \rho\frac{\partial\psi}{\partial\boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}) + \frac{\partial\phi}{\partial\dot{\boldsymbol{\varepsilon}}}(\dot{\boldsymbol{\varepsilon}}) \\ &= \exp(-\mathrm{tr}\,\boldsymbol{\varepsilon})\,(2G\boldsymbol{\varepsilon} + \lambda(\mathrm{tr}\,\boldsymbol{\varepsilon})\boldsymbol{I}) \\ &= 2G\boldsymbol{\varepsilon} + \lambda(\mathrm{tr}\,\boldsymbol{\varepsilon})\boldsymbol{I} + \mathscr{O}\left(|\boldsymbol{\varepsilon}|^2\right) \end{aligned}$$

which describes as expected a Hookean elastic material with the small-strains assumption and (G, λ) are the two Lamé coefficients. The system of equations is closed by coupling with equations of conservation (2a)-(2b).

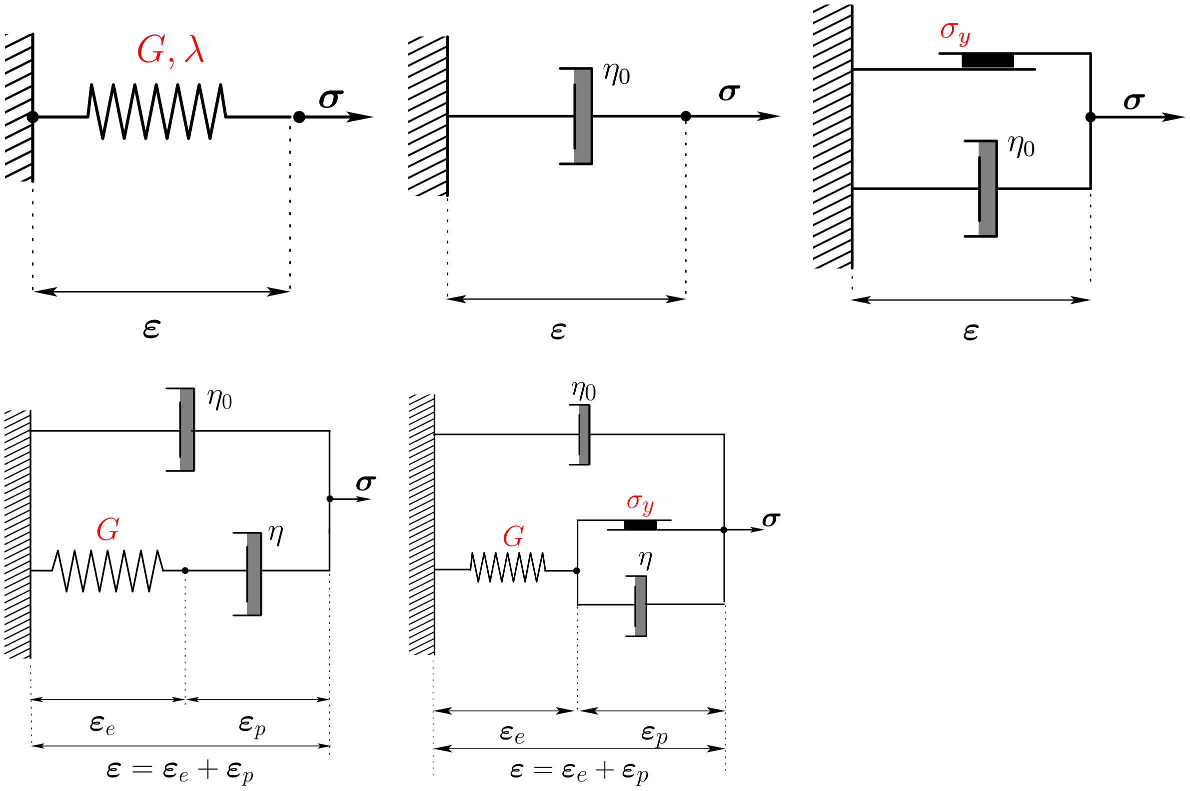

Figure 2: Rheological diagram in small-strains: (top-left) elastic solid ; (top-center) viscous fluid ; (top-right) viscoplastic fluid ; (bottom-left) viscoelastic fluid ; (bottom-center) elastoviscoplastic fluid.

3.2.2. Newtonian fluid

Let $m = 1$ and $\boldsymbol{\alpha} = \boldsymbol{\varepsilon}$. The Newtonian incompressible fluid is described by

$$\begin{cases} \psi(\boldsymbol{\varepsilon}) = 0 \\ \phi(\dot{\boldsymbol{\varepsilon}}) = \mathscr{I}_{\ker(\mathrm{tr})}(\dot{\boldsymbol{\varepsilon}}) + \eta_0 |\dot{\boldsymbol{\varepsilon}}|^2 \end{cases}$$

and is represented on Fig. 2.top-center. The dissipation potential ϕ collects the dashpot element associated to the viscosity η_0 and the incompressibility constraint denoted by $\mathscr{I}_{\ker(\mathrm{tr})}(\dot{\boldsymbol{\varepsilon}})$. Since there is nothing else on the diagram, the free energy ψ is zero. The indicator $\mathscr{I}_{\ker(\mathrm{tr})}(\dot{\boldsymbol{\varepsilon}})$ is zero when $\mathrm{tr}\, \dot{\boldsymbol{\varepsilon}} = 0$ and infinity otherwise. Since $\dot{\boldsymbol{\varepsilon}} = \boldsymbol{D}$, it means that the incompressibility $\mathrm{div}\, \boldsymbol{v} = \mathrm{tr}\, \boldsymbol{D} = 0$ is imposed. Note that the indicator of a convex set is a convex function, so $\mathscr{I}_{\ker(\mathrm{tr})}$ is convex and thus the dissipation potential ϕ satisfies the assumptions of theorem 2. Then, this material satisfies the second principle of thermodynamics. The constitutive equation is obtained from (5a):

$$\boldsymbol{\sigma} = \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}) + \frac{\partial \phi}{\partial \dot{\boldsymbol{\varepsilon}}}(\dot{\boldsymbol{\varepsilon}}) = \partial \mathscr{I}_{\ker(\mathrm{tr})}(\dot{\boldsymbol{\varepsilon}}) + 2\eta_0 \dot{\boldsymbol{\varepsilon}}$$

Using [62, prop. 17, p. 13] for computing the subdifferential of the indicator function, we get the Cauchy stress $\boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta_0 \boldsymbol{D}$. Since $\mathrm{tr}\, \boldsymbol{D} = 0$, remark that the Lagrange multiplier p, associated with the incompressibility constraint, coincides with the physical pressure $-\mathrm{tr}\, \boldsymbol{\sigma}/N$, where $N \geqslant 1$ is the physical space dimension, e.g. $N = 3$. The dissipation writes $\mathscr{D} = 2\eta_0 |\boldsymbol{D}|^2 \geqslant 0$. Finally, the usual incompressible Navier-Stokes equations are obtained by coupling this constitutive equation with equations of conservation (2a)-(2b).

3.2.3. Bingham viscoplastic fluid

Let $m = 1$ and $\boldsymbol{\alpha} = \boldsymbol{\varepsilon}$. The Bingham incompressible viscous fluid is described by

$$\begin{cases} \psi(\boldsymbol{\varepsilon}) = 0 \\ \phi(\dot{\boldsymbol{\varepsilon}}) = \mathscr{I}_{\ker(\mathrm{tr})}(\dot{\boldsymbol{\varepsilon}}) + \eta_0 |\dot{\boldsymbol{\varepsilon}}|^2 + \sigma_y |\dot{\boldsymbol{\varepsilon}}| \end{cases}$$

and is represented on Fig. 2.top-right. The dissipation potential ϕ collects the dashpot element associated to the viscosity η_0 together with the break element associated to the yield stress σ_y and the incompressibility constraint term $\mathscr{I}_{\ker(\mathrm{tr})}(\dot{\boldsymbol{\varepsilon}})$. Since there is nothing else on the diagram, the free energy ψ is zero. The dissipation potential ϕ satisfies the assumptions of theorem 2 and then, this material satisfies the second principle of thermodynamics. Note that the last term of the dissipation potential ϕ, factored by yield stress σ_y, is not differentiable when $\dot{\boldsymbol{\varepsilon}} = 0$ and thus, the constitutive equation (5a) involves a subdifferential:

$$\boldsymbol{\sigma} \in \rho \frac{\partial \psi}{\partial \boldsymbol{\varepsilon}}(\boldsymbol{\varepsilon}) + \frac{\partial \phi}{\partial \dot{\boldsymbol{\varepsilon}}}(\dot{\boldsymbol{\varepsilon}})$$

$$\iff \left\{ \begin{array}{lll} \boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta_0 \dot{\boldsymbol{\varepsilon}} + \sigma_y \dfrac{\dot{\boldsymbol{\varepsilon}}}{|\dot{\boldsymbol{\varepsilon}}|} & & \text{when } \dot{\boldsymbol{\varepsilon}} \neq 0 \\ \boldsymbol{\sigma} = -p\boldsymbol{I} + \boldsymbol{\tau} \text{ and } |\boldsymbol{\tau}| \leqslant \sigma_y & & \text{when } \dot{\boldsymbol{\varepsilon}} = 0 \end{array} \right.$$

The previous development uses $\partial|\dot{\boldsymbol{\varepsilon}}| = \{\boldsymbol{\tau} \; ; \; |\boldsymbol{\tau}| \leqslant 1\}$ when $\dot{\boldsymbol{\varepsilon}} = 0$, see e.g. [61, p. 96]. Finally, using $\dot{\boldsymbol{\varepsilon}} = \boldsymbol{D}$, we get the dissipation $\mathscr{D} = 2\eta_0|\boldsymbol{D}|^2 + \sigma_y|\boldsymbol{D}| \geqslant 0$ and the usual Bingham fluid equations are obtained by coupling this constitutive equation with equations of conservation (2a)-(2b).

3.2.4. Oldroyd-B viscoelastic fluid

As shown on Fig. 2.bottom-left, the total strain splits as $\boldsymbol{\varepsilon} = \boldsymbol{\varepsilon}_e + \boldsymbol{\varepsilon}_p$. This split is very common, and the very conventional subscripts "e" and "p" stand for "elastic" and "plastic" and originate from elastoplasticity. Of the three measures $\boldsymbol{\varepsilon}$, $\boldsymbol{\varepsilon}_e$ and $\boldsymbol{\varepsilon}_p$ of the strain, only two are independent and $(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}_e)$ is chosen as the set of independent thermodynamic state variables, but another choice would have been possible. Let $m = 2$ and $\boldsymbol{\alpha} = (\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}_e)$. The Oldroyd-B viscoelastic fluid is described by

$$\left\{ \begin{array}{l} \psi(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}_e) = \dfrac{G}{\rho_0}|\boldsymbol{\varepsilon}_e|^2 \\ \phi(\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{\varepsilon}}_e) = \mathscr{I}_{\ker(\mathrm{tr})}(\dot{\boldsymbol{\varepsilon}}) + \eta_0|\dot{\boldsymbol{\varepsilon}}|^2 + \eta|\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}_e|^2 \end{array} \right.$$

The free energy ψ collects the spring element associated the elastic modulus G acting with the strain $\dot{\boldsymbol{\varepsilon}}_e$. Note that the bulk modulus λ of the Hookean material is taken as zero (see example 3.2.1). Conversely, the dissipation potential ϕ collects the dashpot element associated to the viscosity η_0 acting with the total strain rate $\dot{\boldsymbol{\varepsilon}}$ together with the dashpot η acting with the strain rate $\dot{\boldsymbol{\varepsilon}}_p = \dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}_e$. Note that the incompressibility constraint term $\mathscr{I}_{\ker(\mathrm{tr})}(\dot{\boldsymbol{\varepsilon}})$ applies only to the total strain rate $\dot{\boldsymbol{\varepsilon}}$, i.e. $\mathrm{tr}\,\dot{\boldsymbol{\varepsilon}} = 0$ whereas $\mathrm{tr}\,\dot{\boldsymbol{\varepsilon}}_e$ remains *a priori* nonzero. From the mass conservation (2a), we get that $\rho = \rho_0$ is constant. The dissipation potential ϕ satisfies the assumptions of theorem 2 and then, this material satisfies the second principle of thermodynamics. The two constitutive equations are obtained from (5a)-(5b):

$$\left\{ \begin{array}{rl} \boldsymbol{\sigma} = & \rho \dfrac{\partial \psi}{\partial \boldsymbol{\varepsilon}} + \dfrac{\partial \phi}{\partial \dot{\boldsymbol{\varepsilon}}} \\ 0 = & \rho \dfrac{\partial \psi}{\partial \boldsymbol{\varepsilon}_e} + \dfrac{\partial \phi}{\partial \dot{\boldsymbol{\varepsilon}}_e} \end{array} \right.$$

$$\iff \left\{ \begin{array}{ll} \boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta_0\dot{\boldsymbol{\varepsilon}} & + 2\eta(\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}_e) \\ 0 = 2G\boldsymbol{\varepsilon}_e & - 2\eta(\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}_e) \end{array} \right.$$

Let $\boldsymbol{\sigma}_e = 2G\boldsymbol{\varepsilon}_e$ be the elastic stress. Combining the two previous equations, we get

$$\left\{ \begin{array}{l} \boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta_0\dot{\boldsymbol{\varepsilon}} + \dot{\boldsymbol{\sigma}}_e \\ \dfrac{\dot{\boldsymbol{\sigma}}_e}{G} + \dfrac{\boldsymbol{\sigma}_e}{\eta} = 2\dot{\boldsymbol{\varepsilon}} \end{array} \right.$$

Note the Lagrange derivative $\dot{\boldsymbol{\sigma}}_e$ in the second equation: it expresses the relaxation of the elastic tensor under the small-strains assumption. In order to obtain the usual Oldroyd-B relaxation equation, we have to replace $\dot{\boldsymbol{\sigma}}_e$ by the upper-convected derivative $\overset{\triangledown}{\boldsymbol{\sigma}}_e$, commonly used in the large-strains assumption. Nevertheless, by doing this, we lose here the warranty from theorem 2: we are not yet able to conclude that the modified model, involving the upper-convected derivative, satisfy the second principle. This crucial question will be addressed in the forthcoming section 4. Finally, using $\dot{\boldsymbol{\varepsilon}} = \boldsymbol{D}$, the usual Oldroyd-B fluid equations are obtained by coupling these constitutive equations with equations of conservation (2a)-(2b).

3.2.5. Elastoviscoplastic fluid

Let $m = 2$ and $\boldsymbol{\alpha} = (\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}_e)$. The elastoviscoplastic fluid is represented on Fig. 2.bottom-center and its structure is similar to those of the Oldroyd-B fluid (Fig. 2.bottom-left): a break element σ_y, acting with the strain rate $\boldsymbol{\varepsilon}_p$ is inserted. The elastoviscoplastic fluid is described by

$$\left\{ \begin{array}{l} \psi(\boldsymbol{\varepsilon}, \boldsymbol{\varepsilon}_e) = \dfrac{G}{\rho_0}|\boldsymbol{\varepsilon}_e|^2 \\ \phi(\dot{\boldsymbol{\varepsilon}}, \dot{\boldsymbol{\varepsilon}}_e) = \mathscr{I}_{\ker(\mathrm{tr})}(\dot{\boldsymbol{\varepsilon}}) + \eta_0|\dot{\boldsymbol{\varepsilon}}|^2 + \varphi(\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}_e) \end{array} \right.$$

where φ is defined for all $\dot{\boldsymbol{\varepsilon}}_p$ by $\varphi(\dot{\boldsymbol{\varepsilon}}_p) = \eta|\dot{\boldsymbol{\varepsilon}}_p|^2 + \sigma_y|\dot{\boldsymbol{\varepsilon}}_p|$. The dissipation potential ϕ satisfies the assumptions of theorem 2 and then, this material satisfies the second principle of thermodynamics. The two constitutive equations are obtained from (5a)-(5b):

$$\left\{\begin{array}{rl} \boldsymbol{\sigma} = & \rho\dfrac{\partial\psi}{\partial\boldsymbol{\varepsilon}} + \dfrac{\partial\phi}{\partial\dot{\boldsymbol{\varepsilon}}} \\ 0 = & \rho\dfrac{\partial\psi}{\partial\boldsymbol{\varepsilon}_e} + \dfrac{\partial\phi}{\partial\dot{\boldsymbol{\varepsilon}}_e} \end{array}\right.$$

$$\Longleftrightarrow \left\{\begin{array}{rll} \boldsymbol{\sigma} & = -p\boldsymbol{I} + 2\eta_0\dot{\boldsymbol{\varepsilon}} & + \partial\varphi(\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}_e) \\ 0 & = 2G\boldsymbol{\varepsilon}_e & - \partial\varphi(\dot{\boldsymbol{\varepsilon}} - \dot{\boldsymbol{\varepsilon}}_e) \end{array}\right.$$

Let $\boldsymbol{\sigma}_e = 2G\boldsymbol{\varepsilon}_e$ be the elastic stress. By combining these two equations, we get [59, p. 5]:

$$\left\{\begin{array}{l} \boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta_0\dot{\boldsymbol{\varepsilon}} + \boldsymbol{\sigma}_e \\ \dfrac{\dot{\boldsymbol{\sigma}}_e}{G} + \max\left(\dfrac{|\mathbf{dev}\,\boldsymbol{\sigma}_e| - \sigma_y}{\eta|\mathbf{dev}\,\boldsymbol{\sigma}_e|}\right)\boldsymbol{\sigma}_e = 2\dot{\boldsymbol{\varepsilon}} \end{array}\right.$$

where $\mathbf{dev}\,\boldsymbol{\tau} = \boldsymbol{\tau} - \mathrm{tr}\,\boldsymbol{\tau}/N$ denotes the deviatoric part of any tensor $\boldsymbol{\tau}$, where $N \geqslant 1$ is the physical space dimension, e.g. $N = 3$. As for the previous Oldroyd-B fluid, note the Lagrange derivative $\dot{\boldsymbol{\sigma}}_e$: the small-strains assumption do not furnish the expected upper-convected derivative $\overset{\triangledown}{\boldsymbol{\sigma}}_e$, specific of large-strains. Finally, using $\dot{\boldsymbol{\varepsilon}} = \boldsymbol{D}$, the elastoviscoplastic fluid equations are obtained by coupling these constitutive equations with equations of conservation (2a)-(2b).

3.3. Discussion

Standard generalized materials provide a clear and easy-to-use environment. Indeed, starting from a rheologic diagram, as on Fig. 2, we are able to specify both the free energy ψ and the dissipation potential ϕ. Then, constitutive equations are automatically obtained from (5a)-(5b) by simple differentiations. The second principle is easy to check: the convexity of ϕ is sufficient. The dissipation potential ϕ could be non-smooth, as for the Bingham fluid model: so this environment supports applications in plasticity, damage and friction, see e.g. [62].

The main drawback of this environment is its small-strains context: for an Oldroyd-B fluid (see paragraph 3.2.4), the differential constitutive equation is obtained with Lagrange derivative $\dot{\boldsymbol{\sigma}}_e$ of the elastic stress. It should be replaced "by hand" by an upper-convected one $\overset{\triangledown}{\boldsymbol{\sigma}}_e$. By doing this, we lose here the warranty from theorem 2 that the model satisfies the second principle.

Paragraph 3.2.4 introduced the Oldroyd-B fluid model with a quadratic Hookean free energy ψ in terms of the small-strains tensor $\boldsymbol{\varepsilon}$ while the free energy is known since the pioneer's work of Grmela [28, eqn (4)] to be related to a nonlinear and non-quadratic neo-Hookean energy, similar to those used in rubbers theory, see Blatz [9]. It requires a large-strains kinematics. Moreover, more nonlinear models, such as the common FENE-P [8] one, could not be described by this small-strains formalism: it also requires a large-strains kinematics.

All theses limitations and open questions will be will be addressed in the next section.

4. Eulerian large-strains extension

This section starts by reviewing the large-strains kinematics in Eulerian frame. Then comes YATE, the extension of the standard generalized material to large-strains in an Eulerian frame. Next, examples involving nonlinear elasticity are presented with details: the neo-Hookean elastic solid followed by the Oldroyd-B, FENE-P, Giesekus and FENE-CR viscoelastic fluids. These examples present both new concise proofs of known results and new results.

4.1. Kinematics

Definition 3 (transformation)**.**
Let $\Omega_0 \subset \mathbb{R}^N$ be an open subset called the *reference configuration*, where $N \geqslant 1$ is the physical space dimension, e.g. $N = 3$.

The trajectory issued at $t = 0$ from a material point $\boldsymbol{X} \in \Omega_0$ is denoted by $(\boldsymbol{\chi}(t, \boldsymbol{X}))_{t \geqslant 0}$ and satisfies:

$$\left\{\begin{array}{ll} \dfrac{\partial\boldsymbol{\chi}}{\partial t}(t, \boldsymbol{X}) = \boldsymbol{v}(t, \boldsymbol{\chi}(t, \boldsymbol{X})),\ \forall t > 0 & \text{(6a)} \\ \boldsymbol{\chi}(0, \boldsymbol{X}) = \boldsymbol{X} & \text{(6b)} \end{array}\right.$$

The first relation (6a) states that the velocity is always tangent to the trajectory while the second one (6b) states that the trajectory passes at time $t = 0$ in $\boldsymbol{X}$, as shown on Fig. 3.top. The existence and unicity of the trajectory $\boldsymbol{\chi}$ as the solution of (6a)-(6b) is guaranteed by the Cauchy-Lipschitz theorem, assuming that the velocity field $\boldsymbol{v}$ is sufficiently regular.

Observe now Fig. 3.center. For a fixed time $t \geqslant 0$, the application $\boldsymbol{X} \in \Omega_0 \longmapsto \boldsymbol{\chi}(t, \boldsymbol{X}) \in \Omega(t)$ is interpreted as the *transformation* from the reference configuration Ω_0 to the current configuration $\Omega(t) = \boldsymbol{\chi}(t, \Omega_0)$ at time t.

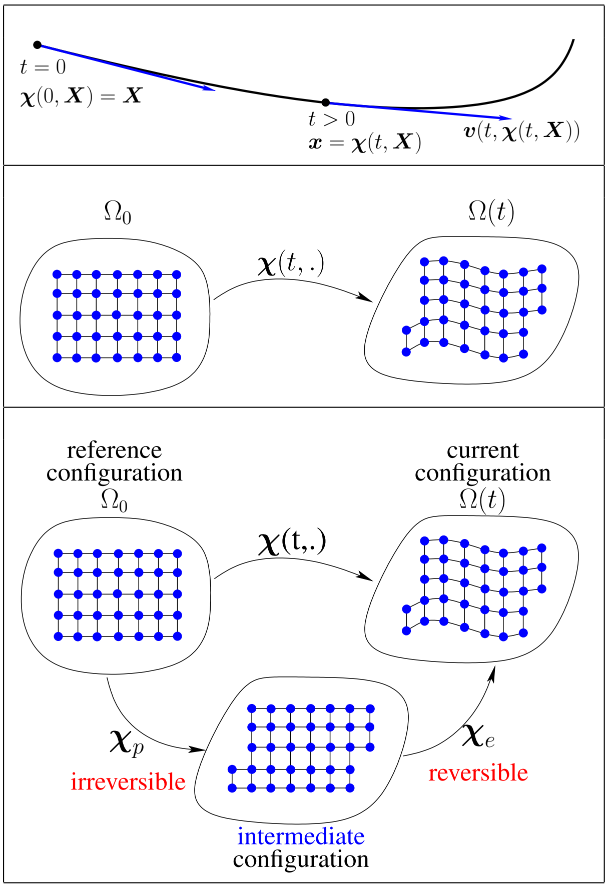

Figure 3: (top) Trajectory $\boldsymbol{\chi}(.,\boldsymbol{X})$ from initial position $\boldsymbol{X}$ to the current one $\boldsymbol{x}=\boldsymbol{\chi}(t,\boldsymbol{X})$; (center) Transformation $\boldsymbol{\chi}(t,.)$ from the reference configuration to the current one ; (bottom) Decomposition $\boldsymbol{\chi}=\boldsymbol{\chi}_e\circ\boldsymbol{\chi}_p$ via the intermediate configuration.

The strain gradient tensor is defined by $\boldsymbol{F}=\nabla\boldsymbol{\chi}=(\partial\chi_i/\partial X_j)_{1\leqslant i,jN}$. Note that some authors adopt an alternative convention for the definition of the gradient of vector-valued functions, as $(\partial\chi_j/\partial X_i)_{1\leqslant i,jN}$ i.e. its transpose, so be sure to double-check it before mixing formulas from different textbooks.

Definition 4 (Cauchy-Green tensor)**.**
The left Cauchy-Green tensor is $\boldsymbol{B}=\boldsymbol{F}\,\boldsymbol{F}^T$. Note that, by construction, $\boldsymbol{B}$ is symmetric positive definite, since the gradient of the transformation is invertible. The right Cauchy-Green tensor $\boldsymbol{C}=\boldsymbol{F}^T\,\boldsymbol{F}$ could also be defined: it is widely used when the strain is uniformly bounded in time, e.g. in solid mechanics, and leads to solve problems in the Lagrangian frame. Here, we focus on the case when the strain is possibly unbounded, e.g. in fluid mechanics, and the Eulerian frame is preferred, together with the left Cauchy-Green tensor $\boldsymbol{B}$.

Definition 5 (strain measures)**.**
There are several ways to develop a strain measure from the left Cauchy-Green tensor $\boldsymbol{B}$. The most common are the left Green-Lagrange strain $\boldsymbol{e}=(\boldsymbol{B}-\boldsymbol{I})/2$ and the left Hencky [32] strain $\boldsymbol{h}=(1/2)\mathbf{log}\,\boldsymbol{B}$. There are many reasons to prefer the left *Hencky* strain to the Green-Lagrange one, see the discussion in paragraph 5.2 below.

Definition 6 (decomposition)**.**
It is convenient to decompose the transformation $\boldsymbol{\chi}$ in several steps when building mathematical models for complex materials. A two-step decomposition is written as $\boldsymbol{\chi}=\boldsymbol{\chi}_e\circ\boldsymbol{\chi}_p$ and is represented on Fig. 3.bottom. The very conventional subscripts "e" and "p" stand for "elastic" and "plastic" and originate from elastoplasticity. In the present context, this refers more generally to reversible and irreversible thermodynamic processes, respectively. Transformation $\boldsymbol{\chi}_p$ is associated with a process in which a part of the energy is irreversibly lost as heat, while the opposite is true for $\boldsymbol{\chi}_e$. Note that even for $\boldsymbol{\chi}_p$, the previous configuration can also be recovered at the cost of additional energy. Thus, the terms reversible/irreversible refer to energy aspects, while the associated configuration is always possibly reversible. By taking the spatial gradient of the previous transformation decomposition, we obtain the multiplicative decomposition of the gradients $\boldsymbol{F}=\boldsymbol{F}_e\boldsymbol{F}_p$ where $\boldsymbol{F}_e=\nabla\boldsymbol{\chi}_e$ and $\boldsymbol{F}_p=\nabla\boldsymbol{\chi}_p$. We are able to define the reversible left Cauchy-Green tensor $\boldsymbol{B}_e=\boldsymbol{F}_e\,\boldsymbol{F}_e^T$ and the reversible left *Hencky* strain $\boldsymbol{h}_e=(1/2)\mathbf{log}\,\boldsymbol{B}_e$. Note that $\boldsymbol{B}_e$ is symmetric positive definite by construction and thus, $\boldsymbol{h}_e$ is well-defined. Its complement, called the irreversible part $\boldsymbol{h}_p$, is such that the following additive decomposition

$$\boldsymbol{h}=\boldsymbol{h}_e+\boldsymbol{h}_p \tag{7a}$$

is satisfied. Conversely, the strain rate splits as:

$$\boldsymbol{D}=\boldsymbol{D}_e+\boldsymbol{D}_p \tag{7b}$$

The following logarithmic corotational derivative was introduced independently in 1991 by Lehmann et al. [41], in 1996 by Reinhardt and Dubey [55, 56] and in 1997 by Xiao et al. [72, p. 92].

Definition 7 (logarithmic corotational derivative)**.**

The *logarithmic corotational derivative* is defined for all symmetric tensor $\boldsymbol{a}$ by:

$$\overset{\circ}{\boldsymbol{a}}^{(\log)} = \dot{\boldsymbol{a}} - \boldsymbol{W}_{\log}(\boldsymbol{a}, \nabla\boldsymbol{v})\boldsymbol{a} + \boldsymbol{a}\boldsymbol{W}_{\log}(\boldsymbol{a}, \nabla\boldsymbol{v})$$

and its associated spin $\boldsymbol{W}_{\log}$ operator, called the *logarithmic spin*, is expressed for all $\boldsymbol{L} \in \mathbb{R}^{N\times N}$ by:

$$\begin{aligned}&\boldsymbol{W}_{\log}(\boldsymbol{a}, \boldsymbol{L})\\ &= \mathbf{skw}(\boldsymbol{L})\\ &\quad - \sum_{i,j=1}^{m_{\boldsymbol{a}}} \kappa_{\log}\left(\lambda_{i,\boldsymbol{a}} - \lambda_{j,\boldsymbol{a}}\right) \boldsymbol{P}_{i,\boldsymbol{a}} \mathbf{sym}(\boldsymbol{L}) \boldsymbol{P}_{j,\boldsymbol{a}}\end{aligned}$$

where, for all $\xi \in \mathbb{R}$:

$$\kappa_{\log}(\xi) = \begin{cases} \dfrac{1}{\tanh\,\xi} - \dfrac{1}{\xi} & \text{when } \xi \neq 0 \\ 0 & \text{otherwise} \end{cases}$$

with $\mathbf{sym}(\boldsymbol{L}) = (\boldsymbol{L} + \boldsymbol{L})/2$, $\mathbf{skw}(\boldsymbol{L}) = (\boldsymbol{L} - \boldsymbol{L})/2$, and where $\lambda_{i,\boldsymbol{a}}$ and $\boldsymbol{P}_{i,\boldsymbol{a}}$, $1 \leqslant i \leqslant m_{\boldsymbol{a}}$, denote the $m_{\boldsymbol{a}}$ distinct eigenvalues and eigenprojectors of $\boldsymbol{a}$, respectively, see e.g. Itskov [38, p. 108].

Proposition 3 (kinematics)**.**

$$\overset{\triangledown}{\boldsymbol{B}} = 0 \tag{8a}$$

$$\overset{\triangledown}{\boldsymbol{B}}_e = -\boldsymbol{D}_p\boldsymbol{B}_e - \boldsymbol{B}_e\boldsymbol{D}_p \tag{8b}$$

$$\overset{\circ}{\boldsymbol{h}}^{(log)} = \boldsymbol{D} \tag{8c}$$

$$\overset{\circ}{\boldsymbol{h}}_e^{(log)} = \boldsymbol{D}_e \textit{ when } \boldsymbol{h}_e \textit{ and } \boldsymbol{D}_p \textit{ commute} \tag{8d}$$

Proof: See [63] pp. 41, 82, 71 and 85, resp. ∎

4.2. Yet another thermodynamic environment

The YATE environment is simply the large-strains extension in Eulerian frame of the standard generalized material (SGM). For clarity, major changes are marked in **bold**. For simplicity, we focuses here on isothermal processes, i.e. θ is constant, see [63] for its coupling with thermal effects.

A YATE material is completely defined by two functions: the free energy ψ and the dissipation potential ϕ. The free energy ψ is assumed to depend upon the set of m thermodynamic *states* denoted by $\boldsymbol{\alpha} = (\alpha_1, \alpha_2, \ldots, \alpha_m)$, $m \geqslant 1$ and the dependency of the function ψ upon the states variables $\boldsymbol{\alpha}$ is denoted as $\psi(\boldsymbol{\alpha})$. By convention $\alpha_1 = \boldsymbol{h}$ is the **left Hencky** strain tensor. When $m \geqslant 2$, $(\alpha_i)_{2\leqslant i\leqslant m}$ represents $m-1$ thermodynamic *internal state variables.* We assume that ψ is objective isotropic separately with respect to all its vector and second-order symmetric tensor arguments α_i, $1 \leqslant i \leqslant m$. Let $\boldsymbol{\delta} = (\delta_1, \delta_2, \ldots, \delta_m)$ be the set of *rates of states.* **From** (8c)**, we have** $\delta_1 = \overset{\circ}{\boldsymbol{h}}^{(log)} = D$ **which is the strain rate tensor**. For all $i \geqslant 2$, when α_i is a scalar field, then $\delta_i = \dot{\alpha}_i$, and otherwise, e.g. when α_i is a vector or tensor field, then δ_i is a **corotational objective** derivatives of the state α_i. The dissipation potential ϕ is assumed to depend upon the rates of states $\boldsymbol{\delta}$, and the dependency of the function ϕ upon the rates variables $\boldsymbol{\delta}$ is denoted as $\phi(\boldsymbol{\delta})$. Optionally, ϕ could also depend upon the states $\boldsymbol{\alpha}$ as parameters, and in that case, it will be denoted as $\phi([\boldsymbol{\alpha}];\ \boldsymbol{\delta})$.

Then, the constitutive equations of the material are given by

$$\begin{cases} \boldsymbol{\sigma} = \rho\dfrac{\partial\psi}{\partial\boldsymbol{h}}(\boldsymbol{\alpha}) + \dfrac{\partial\phi}{\partial\boldsymbol{D}}(\boldsymbol{\delta}), & (i = 1) \qquad (9a) \\ 0 = \rho\dfrac{\partial\psi}{\partial\alpha_i}(\boldsymbol{\alpha}) + \dfrac{\partial\phi}{\partial\delta_i}(\boldsymbol{\delta}), & 2 \leqslant i \leqslant m \qquad (9b) \end{cases}$$

This definition also extends to the case where the dissipation potential ϕ is not differentiable: the previous constitutive equations are simply adjusted by replacing the equal "=" symbol by the belongs to "∈" one.

Theorem 4 (second principle, general case)**.** Assume that the dissipation potential ϕ is nonnegative ($\phi \geqslant 0$), is convex at $\boldsymbol{\delta} = 0$ and vanish in zero, i.e. $\phi(\boldsymbol{\delta}{=}0) = 0$. Then the material described by the two functions ψ and ϕ satisfies the second principle of thermodynamics and the dissipation is given by

$$\mathscr{D} = \sum_{i=0}^{n} \boldsymbol{\delta}_i : \frac{\partial\phi}{\partial\boldsymbol{\delta}_i} \geqslant 0 \tag{10}$$

Proof: see [63, p. 96]. The proof bases on the classical Coleman and Noll [14] procedure while (10) is a direct consequence of the assumptions upon ϕ. ∎

Remark (Onsager symmetry and reciprocal) Since the Hessian $\nabla^2\phi$ is symmetric by construction, the previous model also satisfies a generalized Onsager symmetry (see e.g. [31, 20]). Indeed, this is an extension of the usual Onsager symmetric matrix M case, when $\phi(\boldsymbol{\delta}) = \boldsymbol{\delta}^T M\boldsymbol{\delta}/2$, to the strongly nonlinear case e.g. when ϕ could be non-smooth, as for plasticity.

Then, the following reciprocal of the previous theorem is also true: assume a free energy ψ and a set of constitutive equations satisfying the second principle and the generalized Onsager symmetry. Then, there exists a dissipation potential ϕ such that constitutive equations are expressed by (9) and ϕ satisfies (10).

Finally, the generalized Onsager symmetry could also be relaxed by introducing the Edelen [20] gyroscopic term. It extends to the nonlinear case the situation when the Onsager matrix M is not necessarily symmetric. This feature could be useful for strongly nonlinear problems, e.g. non-associated plasticity or granular matter. For that extension, the reciprocal of the previous theorem is also true in the general non-symmetric case [63, p. 102].

4.3. Examples

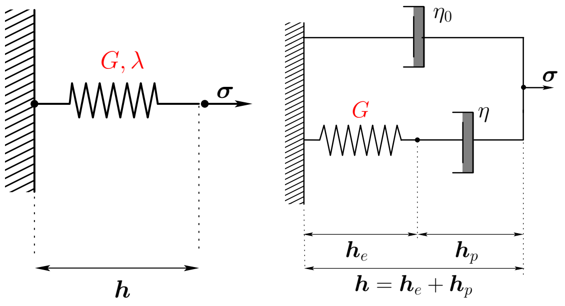

Figure 4: Rheological diagram in large-strains: (left) elastic solid ; (right) Oldroyd-B viscoelastic fluid.

4.3.1. Neo-Hookean elastic solid

The neo-Hookean solid has been introduced in 1971 by Blatz [9, eqn (48)] as a compressible material. Let $m = 1$ and $\boldsymbol{\alpha} = \boldsymbol{h}$. The Eulerian description of this material is given by

$$\begin{cases} \psi(\boldsymbol{h}) = \dfrac{G}{2\rho_0} \operatorname{tr}\left(\mathbf{exp}(2\boldsymbol{h}) - 2\boldsymbol{h} - \boldsymbol{I}\right) \\ \qquad + \dfrac{\lambda}{\rho_0}\left(\exp(\operatorname{tr}\boldsymbol{h}) - \operatorname{tr}\boldsymbol{h} - 1\right) & \text{(11a)} \\ \phi(\boldsymbol{D}) = 0 & \text{(11b)} \end{cases}$$

and is represented on Fig. 4.left. Here, $\rho_0 > 0$ denotes the mass density of the material when in the rest state i.e. when $\boldsymbol{h} = 0$. Also, $G > 0$ and $\lambda > -G$ are the shear and bulk elastic moduli. Note that Blatz [9, eqn (48)] used $K = \lambda + 2G/N$ instead of λ. Since $\xi \in \mathbb{R} \longmapsto \exp\xi - \xi - 1 \geqslant 0$ then $\psi \geqslant 0$ is bounded from below. This material satisfies the second principle of thermodynamics with $\mathscr{D} = 0$. Since $\overset{\circ}{\boldsymbol{h}}{}^{(log)} = \boldsymbol{D}$, then, from the mass conservation (2a), we have $\dot{\rho}/\rho = -\operatorname{div}\boldsymbol{v} = -\operatorname{tr}\boldsymbol{D} = -\operatorname{tr}\overset{\circ}{h}{}^{(log)} = -\operatorname{tr}\boldsymbol{h}$. Next, by integration, we get $\log(\rho/\rho_0) = -\operatorname{tr}\boldsymbol{h}$ i.e. $\rho = \rho_0\exp(-\operatorname{tr}\boldsymbol{h})$. Then, from (9a), we obtain the Eulerian description of the constitutive equation for the neo-Hookean elastic solid:

$$\begin{aligned} \boldsymbol{\sigma} &= \rho\frac{\partial\psi}{\partial\boldsymbol{h}}(\boldsymbol{h}) + \frac{\partial\phi}{\partial\boldsymbol{D}}(\boldsymbol{D}) \\ &= G\exp(-\operatorname{tr}\boldsymbol{h})(\mathbf{exp}(2\boldsymbol{h}) - \boldsymbol{I}) \\ &\quad + \lambda(1 - \exp(-\operatorname{tr}\boldsymbol{h}))\boldsymbol{I} \end{aligned} \tag{12}$$

Note that functions with matrix valued arguments, as ψ here, should be derived with care: for instance, the derivative of the exponential of a matrix $\boldsymbol{m}$ is not the matrix exponential i.e. $\mathbf{exp}'(\boldsymbol{m}) \neq \mathbf{exp}\,\boldsymbol{m}$ while $(\operatorname{tr}\mathbf{exp})'(\boldsymbol{m}) = \mathbf{exp}\,\boldsymbol{m}$, see [63, p. 66], corollaries 3.13 and 3.15. Since $\boldsymbol{h} = \boldsymbol{\varepsilon} + \mathscr{O}\left(|\boldsymbol{\varepsilon}|^2\right)$, we obtain $\boldsymbol{\sigma} = 2G\boldsymbol{\varepsilon} + \lambda(\operatorname{tr}\boldsymbol{\varepsilon})\boldsymbol{I} + \mathscr{O}\left(|\boldsymbol{\varepsilon}|^2\right)$ i.e. the neo-Hookean model extends to large-strains the small-strains Hookean model, as expected, where (G, λ) are the two Lamé coefficients. Finally, the system of equations is closed by coupling the constitutive equation (12) with the kinematic equation (8c) for the evolution of the left Hencky tensor $\boldsymbol{h}$ together with equations of conservation (2a)-(2b). To the best knowledge of the author, this Eulerian formulation of an hyperelastic material in terms of the Hencky tensor is new.

From corollary 2, the zero dissipation case $\mathscr{D} = 0$ leads to the global conservation of the sum of the kinetic and free energies for an isolated isothermal neo-Hookean solid. The ball of Fig. 1 would bounce indefinitely: this idealized situation will be improved by the introduction of a dissipative mechanism.

4.3.2. Oldroyd-B viscoelastic fluid

Similarly to the small-strains case, Fig. 4.right represent the model. From (7a), the total strain splits as $\boldsymbol{h} = \boldsymbol{h}_e + \boldsymbol{h}_p$. Let $m = 2$ and $\boldsymbol{\alpha} = (\boldsymbol{h}, \boldsymbol{h}_e)$. The Oldroyd-B viscoelastic fluid [49] is described in terms of the two independent state variables $(\boldsymbol{h}, \boldsymbol{h}_e)$

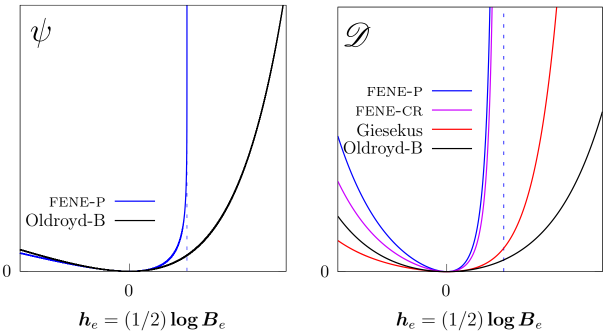

Figure 5: Free energy ψ (left) and dissipation $\mathscr{D}$ (right) for the FENE-P, FENE-CR, Giesekus and Oldroyd-B models ($N=1, \eta_0=0, \alpha=1/2, \beta=1/3$).

by

$$\left\{\begin{aligned} &\psi(\boldsymbol{h},\boldsymbol{h}_e) = \frac{G}{2\rho_0}\mathrm{tr}\,(\mathbf{exp}(2\boldsymbol{h}_e) - 2\boldsymbol{h}_e - \boldsymbol{I}) && \text{(13a)} \\ &\phi([\boldsymbol{h}_e];\boldsymbol{D},\boldsymbol{D}_e) = \mathscr{I}_{\ker(\mathrm{tr})}(\boldsymbol{D}) + \eta_0|\boldsymbol{D}|^2 \\ &\qquad\qquad + \eta|\mathbf{exp}(\boldsymbol{h}_e)(\boldsymbol{D}-\boldsymbol{D}_e)|^2 && \text{(13b)} \end{aligned}\right.$$

The free energy ψ is the compressible neo-Hookean expression (11a) simplified with $\lambda = 0$, and applied to the reversible strain $\boldsymbol{h}_e$, see Fig. 5.left. Conversely, the dissipation potential ϕ is similar to the small-strains case, except a weighted norm with $\mathbf{exp}\,\boldsymbol{h}_e$ for the last term. While ϕ depends upon the two rate variables $\boldsymbol{D}$ and $\boldsymbol{D}_e$, the state variable $\boldsymbol{h}_e$ is here considered as a parameter for ϕ and its dependency is denoted by square brackets. Since $\mathbf{exp}\,\boldsymbol{h}_e$ is positive definite, the dissipation potential ϕ satisfies the assumptions of theorem 4 and then, the Oldroyd-B viscoelastic fluid model satisfies the second principle of thermodynamics. Note that, since the material is incompressible, from (2a), we get $\dot{\rho} = 0$ and then the density $\rho = \rho_0$ is constant. Also $\mathrm{tr}\,\boldsymbol{h} = 0$ whereas $\mathrm{tr}\,\boldsymbol{h}_e$ remains *a priori* nonzero. The two constitutive equations are obtained from (5a)-(5b):

$$\left\{\begin{aligned} \boldsymbol{\sigma} &= \rho\frac{\partial\psi}{\partial\boldsymbol{h}} + \frac{\partial\phi}{\partial\boldsymbol{D}} \\ 0 &= \rho\frac{\partial\psi}{\partial\boldsymbol{h}_e} + \frac{\partial\phi}{\partial\boldsymbol{D}_e} \end{aligned}\right.$$

$$\iff \left\{\begin{aligned} \boldsymbol{\sigma} &= -p\boldsymbol{I} + 2\eta_0\boldsymbol{D} \\ &\quad + \eta\big(\mathbf{exp}(2\boldsymbol{h}_e)(\boldsymbol{D}-\boldsymbol{D}_e) \\ &\qquad + (\boldsymbol{D}-\boldsymbol{D}_e)\mathbf{exp}(2\boldsymbol{h}_e)\big) \\ 0 &= G\big(\mathbf{exp}(2\boldsymbol{h}_e) - \boldsymbol{I}\big) \\ &\quad - \eta\big(\mathbf{exp}(2\boldsymbol{h}_e)(\boldsymbol{D}-\boldsymbol{D}_e) \\ &\qquad + (\boldsymbol{D}-\boldsymbol{D}_e)\mathbf{exp}(2\boldsymbol{h}_e)\big) \end{aligned}\right.$$

after expanding ψ as in paragraph 4.3.1

$$\iff \left\{\begin{aligned} \boldsymbol{\sigma} &= -p\boldsymbol{I} + 2\eta_0\boldsymbol{D} + G(\boldsymbol{B}_e - \boldsymbol{I}) \\ 0 &= G(\boldsymbol{B}_e - \boldsymbol{I}) - \eta(\boldsymbol{B}_e\boldsymbol{D}_p + \boldsymbol{D}_p\boldsymbol{B}_e) \end{aligned}\right.$$

after using $\boldsymbol{B}_e = \mathbf{exp}(2\boldsymbol{h}_e)$ and $\boldsymbol{D}_p = \boldsymbol{D} - \boldsymbol{D}_e$ from (7b)

$$\iff \left\{\begin{aligned} &\boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta_0\boldsymbol{D} + G(\boldsymbol{B}_e - \boldsymbol{I}) \\ &\frac{\eta}{G}\overset{\triangledown}{\boldsymbol{B}_e} + \boldsymbol{B}_e = \boldsymbol{I} \end{aligned}\right.$$

after using the kinematic relation (8b). We immediately recognize the Oldroyd-B model expressed in terms of the conformation tensor, originally introduced in 1966 by Giesekus [25, eqn (23)] for the formulation of the Oldroyd-B model. Note that Giesekus [25] introduced a dimensional conformation tensor denoted by $\langle\boldsymbol{rr}\rangle$ and proportional to $\boldsymbol{B}_e$ with a r_0^2 factor, where r_0 denotes a microstructure length in a reference configuration, i.e. $\boldsymbol{B}_e = r_0^{-2}\langle\boldsymbol{rr}\rangle$. In consequence, the reversible left Cauchy-Green tensor $\boldsymbol{B}_e$ identifies as the dimensionless **conformation tensor** used in the context of viscoelastic fluids. Note that, unlike the small-strains case from paragraph 3.2.4, here we directly obtain the upper-convected derivative of the Oldroyd-B model: there is no more Lagrangian derivative to replace "by hand". Also, the simple convexity of ϕ is sufficient to conclude that this model satisfies the second principle of thermodynamics.

Few lines ahead, we obtained $\boldsymbol{B}_e\boldsymbol{D}_p + \boldsymbol{D}_p\boldsymbol{B}_e = (G/\eta)(\boldsymbol{B}_e - \boldsymbol{I})$ which means that $\boldsymbol{D}_p$ and $\boldsymbol{B}_e$ share the same eigenspace (see [63, p. 60], lemma 3.8) and then commute. Then $\boldsymbol{D}_p = (G/(2\eta))(\boldsymbol{I} - \boldsymbol{B}_e^{-1})$ and the kinematic relation (8d) applies: we get $\overset{\circ\,(log)}{\boldsymbol{h}_e} = \boldsymbol{D}_e = \boldsymbol{D} - \boldsymbol{D}_p$. Combining these two last relations and using $\boldsymbol{B}_e^{-1} = \mathbf{exp}(-2\boldsymbol{h}_e)$, we obtain the following equivalent formulation of the Oldroyd-B model in terms of the reversible left Hencky strain $\boldsymbol{h}_e$:

$$\left\{\begin{aligned} &\boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta_0\boldsymbol{D} + G(\mathbf{exp}(2\boldsymbol{h}_e) - \boldsymbol{I}) && \text{(14a)} \\ &\overset{\circ\,(log)}{\boldsymbol{h}_e} + \frac{G}{2\eta}(\boldsymbol{I} - \mathbf{exp}(-2\boldsymbol{h}_e)) = \boldsymbol{D} && \text{(14b)} \end{aligned}\right.$$

Recall that the reversible left Hencky strain $\boldsymbol{h}_e = (1/2)\mathbf{log}\,\boldsymbol{B}_e$ i.e. it coincides with the **logarithm of the conformation tensor** $\boldsymbol{B}_e$, up to a 1/2 factor. This formulation is thus of major interest, not only from theoretical reason, but also it is already widely used by most numerical algorithms for solving the Oldroyd-B model.

At the limit $G/\eta \to 0$, the constitutive equation (14b) reduces to the kinematic relation (8c), i.e. $\boldsymbol{h}_e = \boldsymbol{h}$. When, moreover $\eta_0 = 0$, then the Oldroyd-B viscoelastic fluid reduces to an incompressible neo-Hookean elastic solid.

From (10), the **dissipation** writes (see Fig. 5.right):

$$
\begin{aligned}
\mathscr{D} &= \frac{\partial\phi}{\partial \boldsymbol{D}} : \boldsymbol{D} + \frac{\partial\phi}{\partial \boldsymbol{D}_e} : \boldsymbol{D}_e \\
&= 2\eta_0|\boldsymbol{D}|^2 + 2\eta\,|\mathbf{exp}(\boldsymbol{h}_e)\boldsymbol{D}_p|^2 \\
&\quad \text{after expansion of } \phi \\
&= 2\eta_0|\boldsymbol{D}|^2 + \frac{G^2}{2\eta}\mathrm{tr}\big(\boldsymbol{B}_e + \boldsymbol{B}_e^{-1} - 2\boldsymbol{I}\big) \\
&\quad \text{using the previous expression of } \boldsymbol{D}_p \\
&= 2\eta_0|\boldsymbol{D}|^2 \\
&\quad + \frac{G^2}{2\eta}\mathrm{tr}\big(\mathbf{exp}(2\boldsymbol{h}_e) + \mathbf{exp}(-2\boldsymbol{h}_e) - 2\boldsymbol{I}\big) \qquad (15)
\end{aligned}
$$

Observe that $e^{2\xi} + e^{-2\xi} - 2 \geqslant 0$ for any $\xi \in \mathbb{R}$ and then $\mathscr{D} \geqslant 0$. Then, in addition to theorem 4, we obtain a second and direct proof that the Oldroyd-B viscoelastic fluid model satisfies the second principle of thermodynamics. This expression of $\mathscr{D}$ is in agreement with those that could be obtained from the Poisson bracket formalism by Beris and Edwards [5], see appendix Appendix B. Moreover, we directly conclude from (15) that $\mathscr{D} \geqslant 0$ for any vector field $\boldsymbol{v}$ and any tensor $\boldsymbol{h}_e$ while Beris and Edwards [5] used the expression of $\mathscr{D}$ in terms of $\boldsymbol{B}_e$ instead, and had in addition to prove that $\boldsymbol{B}_e$ remains positive definite during all its evolution, which is not obvious, see Hulsen [35] and Beris and Edwards [6, p. 272-281].

Finally, the following **entropy estimate** for an isolated isothermal Oldroyd-B fluid is obtained by applying corollary 2, replacing in (4) the symbols ψ and $\mathscr{D}$ by their expressions from (13a) and (15) respectively:

$$
\begin{aligned}
&\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho\frac{|\boldsymbol{v}|^2}{2} + \frac{G}{2}\mathrm{tr}\left(\boldsymbol{B}_e - \mathbf{log}\,\boldsymbol{B}_e - \boldsymbol{I}\right) \\
&\quad + \int_\Omega 2\eta_0|\boldsymbol{D}|^2 + \frac{G^2}{2\eta}\mathrm{tr}\big(\boldsymbol{B}_e + \boldsymbol{B}_e^{-1} - 2\boldsymbol{I}\big) = 0 \qquad (16)
\end{aligned}
$$

Recall that this relation expresses that the sum of the kinetic and free energies decreases and is bounded for an isolated system. It has been established for the first time in 2007 by Hu and Lelièvre [34, eqn (3.13)]. Unlike these authors, who had to develop a specific and technical proof, this estimate here follows directly from corollary 2, which has general applicability.

4.3.3. FENE-P *viscoelastic fluid*

Introduced in 1980 by Bird et al. [8], this model extends the Oldroyd-B one by introducing a more realistic non neo-Hookean energy, see Fig. 5.left. This model is obtained with $n = 2$ and $\boldsymbol{\alpha} = (\boldsymbol{h}, \boldsymbol{h}_e)$ with

$$
\begin{aligned}
&\psi(\boldsymbol{h}, \boldsymbol{h}_e) \\
&\quad = \frac{G}{\rho_0}\left(\frac{N}{2\beta}\log\left(\frac{1-\beta}{1 - \dfrac{\beta}{N}\,\mathrm{tr}\,\mathbf{exp}(2\boldsymbol{h}_e)}\right) - \frac{\mathrm{tr}\,\boldsymbol{h}_e}{1-\beta}\right) \\
&\qquad + \mathscr{I}_{[0,N/\beta[}\left(\mathrm{tr}\,\mathbf{exp}(2\boldsymbol{h}_e)\right) \qquad (17a)
\end{aligned}
$$

$$
\begin{aligned}
&\phi([\boldsymbol{h}_e];\ \boldsymbol{D}, \boldsymbol{D}_e) = \mathscr{I}_{\ker(\mathrm{tr})}(\boldsymbol{D}) + \eta_0|\boldsymbol{D}|^2 \\
&\qquad + \eta\,|\mathbf{exp}(\boldsymbol{h}_e)(\boldsymbol{D} - \boldsymbol{D}_e)|^2 \qquad (17b)
\end{aligned}
$$

where $\beta \in]0,1[$ is the new parameter of the model. With the notations of Bird et al. [8], the dimensionless measure of the extensibility of the dumbells expresses $L^2 = N/\beta$. Note that $\psi \geqslant 0$ is bounded from below. Observe that, by a first order expansion of the log for small β, the free energy ψ could be extended by continuity at the limit $\beta = 0$: in that case, the FENE-P viscoelastic fluid model reduces to the Oldroyd-B one. Since the dissipation potential ϕ is unchanged from the Oldroyd-B model,, theorem 4 applies and then, the FENE-P viscoelastic fluid model satisfies the second principle of thermodynamics.

As in the previous example, the elastic stress $\boldsymbol{\sigma}_e = \rho\,\psi'(\boldsymbol{h}_e)$ should be computed with care. Assuming $\mathrm{tr}\,\mathbf{exp}(2\boldsymbol{h}_e) < N/\beta$, let us compute the Gâteau derivative of ψ at $\boldsymbol{h}_e$ in an arbitrarily direction $\boldsymbol{d}$:

$$\begin{aligned}
&\rho\,\psi'(\boldsymbol{h}_e):\boldsymbol{d}\\
&= \lim_{\varepsilon\to 0}\ \rho\,\frac{\psi(\boldsymbol{h}_e+\varepsilon\boldsymbol{d})-\psi(\boldsymbol{h}_e)}{\varepsilon}\\
&= \lim_{\varepsilon\to 0}\ \frac{GN}{\beta\varepsilon}\left(-\log\left(1-\frac{\beta}{N}\operatorname{tr}\mathbf{exp}(2(\boldsymbol{h}_e+\varepsilon\boldsymbol{d}))\right)\right.\\
&\qquad\qquad \left.+\log\left(1-\frac{\beta}{N}\operatorname{tr}\mathbf{exp}(2\boldsymbol{h}_e)\right)\right)\\
&\qquad -\frac{G}{1-\beta}\boldsymbol{I}:\boldsymbol{d}\\
&= G\left(\frac{\mathbf{exp}(2\boldsymbol{h}_e)}{1-\dfrac{\beta}{N}\operatorname{tr}\mathbf{exp}(2\boldsymbol{h}_e)}-\frac{\boldsymbol{I}}{1-\beta}\right):\boldsymbol{d}
\end{aligned}$$

by differentiation of log and from $(\operatorname{tr}\mathbf{exp})'(\boldsymbol{m})=\mathbf{exp}\boldsymbol{m}$, for any matrix $\boldsymbol{m}$. Then

$$\boldsymbol{\sigma}_e = G\left(\frac{\mathbf{exp}(2\boldsymbol{h}_e)}{1-\dfrac{\beta}{N}\operatorname{tr}\mathbf{exp}(2\boldsymbol{h}_e)}-\frac{\boldsymbol{I}}{1-\beta}\right) \tag{18a}$$

Observe that when $\beta=0$, the elastic stress reduces to $\boldsymbol{\sigma}_e = G(\mathbf{exp}(2\boldsymbol{h}_e)-\boldsymbol{I}) = G(\boldsymbol{B}_e-\boldsymbol{I})$ i.e. to the case of the Oldroyd-B model, as expected. Observe also from (18a) that $\boldsymbol{\sigma}_e$ and $\boldsymbol{h}_e$ share the same eigensystem and then commute. The two constitutive equations are obtained from (5a)-(5b):

$$\left\{\begin{aligned}
\boldsymbol{\sigma} &= \rho\frac{\partial\psi}{\partial\boldsymbol{h}}+\frac{\partial\phi}{\partial\boldsymbol{D}}\\
0 &= \rho\frac{\partial\psi}{\partial\boldsymbol{h}_e}+\frac{\partial\phi}{\partial\boldsymbol{D}_e}
\end{aligned}\right.$$

$$\iff \left\{\begin{aligned}
\boldsymbol{\sigma} \ &= -p\boldsymbol{I}+2\eta_0\boldsymbol{D}\\
&\quad +\eta\big(\mathbf{exp}(2\boldsymbol{h}_e)(\boldsymbol{D}-\boldsymbol{D}_e)\\
&\qquad +(\boldsymbol{D}-\boldsymbol{D}_e)\mathbf{exp}(2\boldsymbol{h}_e)\big)\\
0 \ &= \boldsymbol{\sigma}_e-\eta\big(\mathbf{exp}(2\boldsymbol{h}_e)(\boldsymbol{D}-\boldsymbol{D}_e)\\
&\qquad +(\boldsymbol{D}-\boldsymbol{D}_e)\mathbf{exp}(2\boldsymbol{h}_e)\big)
\end{aligned}\right.$$

after expanding, as in paragraph 4.3.2

$$\iff \left\{\begin{aligned}
\boldsymbol{\sigma} &= -p\boldsymbol{I}+2\eta_0\boldsymbol{D}+\boldsymbol{\sigma}_e\\
\boldsymbol{\sigma}_e &= \eta(\mathbf{exp}(2\boldsymbol{h}_e)\boldsymbol{D}_p+\boldsymbol{D}_p\mathbf{exp}(2\boldsymbol{h}_e))
\end{aligned}\right.$$

after using $\boldsymbol{D}_p=\boldsymbol{D}-\boldsymbol{D}_e$ from (7b). Since $\boldsymbol{\sigma}_e$ and $\boldsymbol{h}_e$ share the same eigensystem, then, the last relation expresses that both $\boldsymbol{D}_p$, $\boldsymbol{\sigma}_e$ and $\boldsymbol{h}_e$ share the same eigensystem and then commute. Then, the last relation writes also as $\boldsymbol{\sigma}_e = 2\eta\,\mathbf{exp}(2\boldsymbol{h}_e)\boldsymbol{D}_p$. Also, the kinematic relation (8d) applies: we get $\overset{\circ}{\boldsymbol{h}}{}_e^{(log)} = \boldsymbol{D}_e = \boldsymbol{D}-\boldsymbol{D}_p$ i.e. $\boldsymbol{D}_p = \boldsymbol{D}-\overset{\circ}{\boldsymbol{h}}{}_e^{(log)}$. Replacing in the previous expression of $\boldsymbol{\sigma}_e$, we get

$$\boldsymbol{\sigma}_e = 2\eta\,\mathbf{exp}(2\boldsymbol{h}_e)\left(\boldsymbol{D}-\overset{\circ}{\boldsymbol{h}}{}_e^{(log)}\right)$$

Then, the two constitutive equations become, after rearrangements:

$$\left\{\begin{aligned}
&\boldsymbol{\sigma} = -p\boldsymbol{I}+2\eta_0\boldsymbol{D}+\boldsymbol{\sigma}_e && (18\text{b})\\
&\overset{\circ}{\boldsymbol{h}}{}_e^{(log)} + \frac{1}{2\eta}\mathbf{exp}(-2\boldsymbol{h}_e)\boldsymbol{\sigma}_e = \boldsymbol{D} && (18\text{c})
\end{aligned}\right.$$

Together with (18a), this system represents the formulation of the FENE-P model in terms of the reversible left Hencky strain $\boldsymbol{h}_e$, i.e. the logarithm of the conformation tensor. It is widely used for numerical simulations. Instead of (8d), we could use the kinematic relation (8b) for replacing $\boldsymbol{D}_p$, and obtain the formulation of the FENE-P model in terms of the reversible left Cauchy-Green tensor $\boldsymbol{B}_e$, i.e. the conformation tensor:

$$\left\{\begin{aligned}
&\boldsymbol{\sigma} = -p\boldsymbol{I}+2\eta_0\boldsymbol{D}+G\left(\frac{\boldsymbol{B}_e}{1-\dfrac{\beta}{N}\operatorname{tr}\boldsymbol{B}_e}-\frac{\boldsymbol{I}}{1-\beta}\right) && (19\text{a})\\
&\frac{\eta}{G}\,\overset{\triangledown}{\boldsymbol{B}}_e + \frac{\boldsymbol{B}_e}{1-\dfrac{\beta}{N}\operatorname{tr}\boldsymbol{B}_e} = \frac{\boldsymbol{I}}{1-\beta} && (19\text{b})
\end{aligned}\right.$$

Observe that when $\beta=0$, the FENE-P constitutive equations nicely reduce to the Oldroyd-B model, as expected. Formulation (19a)-(19b) is also widely used when considering the FENE-P model for numerical simulations, see e.g. Purnode and Legat [54], eqn (10), where $\boldsymbol{B}_e$ is denoted as $\boldsymbol{A}$. Its original formulation from Bird et al. [8], eqns (5) and (9), is also based on a conformation tensor of the microstructure that is simply proportional to $\boldsymbol{B}_e$.

At the limit $G/\eta\to 0$, the constitutive equation (18c) reduces to the kinematic relation (8c), i.e. $\boldsymbol{h}_e=\boldsymbol{h}$. When, moreover $\eta_0=0$, then the FENE-P viscoelastic fluid reduces to an incompressible Gent [22] elastic solid: its constitutive equations are given by (18a)-(18b) with $\boldsymbol{h}_e=\boldsymbol{h}$.

Finally, from (10), the **dissipation** writes (see Fig. 5.right):

$$\begin{aligned}
\mathscr{D} &= 2\eta_0|\boldsymbol{D}|^2+\frac{1}{2\eta}\operatorname{tr}\left(\boldsymbol{B}_e^{-1}\boldsymbol{\sigma}_e^2\right)\\
&= 2\eta_0|\boldsymbol{D}|^2\\
&\quad +\frac{G^2}{2\eta}\operatorname{tr}\left(\boldsymbol{B}_e^{-1}\left(\frac{\boldsymbol{B}_e}{1-\dfrac{\beta}{N}\operatorname{tr}\boldsymbol{B}_e}-\frac{\boldsymbol{I}}{1-\beta}\right)^2\right)
\end{aligned} \tag{20}$$

Thus $\mathscr{D} \geqslant 0$ since $\boldsymbol{B}_e^{-1} = \mathbf{exp}(-2\boldsymbol{h}_e) > 0$, which furnishes another and direct proof that the FENE-P viscoelastic fluid model satisfies the second principle of thermodynamics.

Finally, the following **entropy estimate** for an isolated isothermal FENE-P fluid is directly obtained by applying corollary 2, replacing in (4) the symbols ψ and $\mathscr{D}$ by their expressions from (17a) and (20) respectively:

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho\frac{|\boldsymbol{v}|^2}{2}\\ &\quad+\frac{G}{2}\left(\frac{N}{\beta}\log\left(\frac{1-\beta}{1-\dfrac{\beta}{N}\operatorname{tr}\boldsymbol{B}_e}\right)-\frac{\operatorname{tr}\mathbf{log}\,\boldsymbol{B}_e}{1-\beta}\right)\\ &+\int_\Omega 2\eta_0|\boldsymbol{D}|^2\\ &\quad+\frac{G^2}{2\eta}\operatorname{tr}\left(\boldsymbol{B}_e^{-1}\left(\frac{\boldsymbol{B}_e}{1-\dfrac{\beta}{N}\operatorname{tr}\boldsymbol{B}_e}-\frac{\boldsymbol{I}}{1-\beta}\right)^2\right)=0 \qquad (21)\end{aligned}$$

Relation (21) has been established for the first time in 2007 by Hu and Lelièvre [34, p. 914]. Note that these authors used the formulation of the FENE-P model introduced by Housiadas and Beris [33]: up to a scaling procedure of the conformation tensor discussed in paragraph 4.3.5 below, their final estimate [34, p. 914] coincides exactly with (21).

4.3.4. The Giesekus model

The Giesekus [26] model is obtained in the YATE environment by using the neo-Hookean free energy ψ from (13a) unchanged from the Oldroyd-B model and replacing its potential ϕ as:

$$\begin{aligned}\phi([\boldsymbol{h}_e];\ \boldsymbol{D},\boldsymbol{D}_e) &= \mathscr{I}_{\ker(\mathrm{tr})}(\boldsymbol{D}) + \eta_0|\boldsymbol{D}|^2\\ &\quad+\eta\left|\mathbf{exp}(\boldsymbol{h}_e)\mathbb{A}^{-\frac{1}{2}}:(\boldsymbol{D}-\boldsymbol{D}_e)\right|^2 \qquad (22a)\end{aligned}$$

where $\mathbb{A}$ is the fourth-order *mobility* tensor defined for all second order tensors $\boldsymbol{\tau}$ by

$$\mathbb{A}:\boldsymbol{\tau} = \alpha\,\mathbf{sym}(\boldsymbol{B}_e\boldsymbol{\tau}) + (1-\alpha)\boldsymbol{\tau} \qquad (22b)$$

where $\alpha \in [0,1]$ is a parameter of the Giesekus model. When $\alpha = 0$, this model reduces to the Oldroyd-B one. Note that, since both $\boldsymbol{B}_e = \mathbf{exp}(2\boldsymbol{h}_e)$ and $\alpha\boldsymbol{B}_e + (1-\alpha)\boldsymbol{I}$ are symmetric definite positive, then $\boldsymbol{\tau}:(\mathbb{A}:\boldsymbol{\tau}) \geqslant c_0|\boldsymbol{\tau}|^2$ for any $\boldsymbol{\tau}$, for some constant $c_0 > 0$ that depends only upon α and $\boldsymbol{B}_e$, and then $\mathbb{A}$ is symmetric definite positive for all $\alpha \in [0,1]$. Then ϕ is convex and this model satisfies the second principle. The concept of *mobility* was introduced by Giesekus [26] as a second-order tensor. It is presented here for convenience as a fourth-order tensor, i.e. as a linear application over second-order tensors. Since ψ is unchanged from the Oldroyd-B model, the elastic stress still writes $\boldsymbol{\sigma}_e = G(\boldsymbol{B}_e - \boldsymbol{I})$. The two constitutive equations are obtained from (5a)-(5b) with ψ and ϕ given by (13a) and (22a) respectively:

$$\left\{\begin{aligned}\boldsymbol{\sigma}\ &= -p\boldsymbol{I} + 2\eta_0\boldsymbol{D} + \boldsymbol{\sigma}_e && (23a)\\ \boldsymbol{\sigma}_e &= 2\eta\,\mathbf{exp}(2\boldsymbol{h}_e)\,\mathbb{A}^{-1}:\boldsymbol{D}_p && (23b)\end{aligned}\right.$$

where we used the commutation between $\boldsymbol{D}_p$ and $\boldsymbol{B}_e$. Inverting the mobility tensor $\mathbb{A}$, the second constitutive equation (23b) writes equivalently as:

$$\boldsymbol{D}_p = \frac{1}{2\eta}\mathbf{exp}(-2\boldsymbol{h}_e)\,\mathbb{A}:\boldsymbol{\sigma}_e \qquad (24)$$

Using the kinematic relation (8d), we obtain from (24) a differential constitutive equation in terms of $\boldsymbol{h}_e$:

$$\begin{aligned}&\overset{\circ}{\boldsymbol{h}}{}^{(log)} + \frac{1}{2\eta}\mathbf{exp}(-2\boldsymbol{h}_e)\,\mathbb{A}:\boldsymbol{\sigma}_e = \boldsymbol{D} && (25a)\\ \Longleftrightarrow\ &\overset{\circ}{\boldsymbol{h}}{}^{(log)} + \frac{G}{2\eta}\left\{\boldsymbol{I} + \alpha\left(\mathbf{exp}(2\boldsymbol{h}_e) - \boldsymbol{I}\right)\right\}\\ &\qquad\times\left(\boldsymbol{I} - \mathbf{exp}(-2\boldsymbol{h}_e)\right) = \boldsymbol{D} && (25b)\end{aligned}$$

Conversely, using the kinematic relation (8b), we obtain from (24) a differential constitutive equation in terms of $\boldsymbol{B}_e$:

$$\begin{aligned}&\overset{\triangledown}{\boldsymbol{B}}_e + \frac{1}{\eta}\mathbb{A}:\boldsymbol{\sigma}_e = 0 && (26a)\\ \Longleftrightarrow\ &\frac{\eta}{G}\overset{\triangledown}{\boldsymbol{B}}_e + \{\boldsymbol{I}+\alpha(\boldsymbol{B}_e-\boldsymbol{I})\}\,(\boldsymbol{B}_e-\boldsymbol{I}) = 0 && (26b)\end{aligned}$$

which coincides with eqns (10) and (34)-(35) of the Giesekus [26] model. Furthermore, the reversible left Cauchy-Green tensor $\boldsymbol{B}_e$ coincides with the **conformation tensor** discussed by Giesekus [26, p. 70] as "*characterizing the configurational state of the different kinds of network structures present in the concentrated solution or melt*".

From (10), the **dissipation** writes (see Fig. 5.right):

$$\begin{aligned}\mathscr{D} &= 2\eta_0|\boldsymbol{D}|^2 + 2\eta\operatorname{tr}\left(\boldsymbol{B}_e\left(\mathbb{A}^{-1}:\boldsymbol{D}_p\right)\boldsymbol{D}_p\right)\\ &= 2\eta_0|\boldsymbol{D}|^2 + \frac{1}{2\eta}\operatorname{tr}\left(\boldsymbol{B}_e^{-1}\boldsymbol{\sigma}_e\left(\mathbb{A}:\boldsymbol{\sigma}_e\right)\right)\\ &= 2\eta_0|\boldsymbol{D}|^2\\ &\quad+\frac{G^2}{2\eta}\operatorname{tr}\left(\{(1-\alpha)\boldsymbol{B}_e^{-1}+\alpha\boldsymbol{I}\}\,(\boldsymbol{B}_e-\boldsymbol{I})^2\right) \qquad (27)\end{aligned}$$

where we used (24) and expanded the mobility $\mathbb{A}$ and the elastic stress $\boldsymbol{\sigma}_e = G(\boldsymbol{B}_e - \boldsymbol{I})$. Thus, we directly check here that $\mathscr{D} \geqslant 0$ since $\boldsymbol{B}_e^{-1} = \mathbf{exp}(-2\boldsymbol{h}_e)$ is symmetric definite positive.

Finally, the **entropy estimate** for the Giesekus model follows from corollary 2 by using ψ and $\mathscr{D}$ from (13a) and (27), respectively:

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho\frac{|\boldsymbol{v}|^2}{2} + \frac{G}{2}\mathrm{tr}\left(\boldsymbol{B}_e - \mathbf{log}\,\boldsymbol{B}_e - \boldsymbol{I}\right)\\ &+ \int_\Omega 2\eta_0|\boldsymbol{D}|^2\\ &\quad + \frac{G^2}{2\eta}\mathrm{tr}\left(\{(1-\alpha)\boldsymbol{B}_e^{-1} + \alpha\boldsymbol{I}\}(\boldsymbol{B}_e - \boldsymbol{I})^2\right)\\ &= 0 \end{aligned} \tag{28}$$

A similar estimate was established in 2011 by Masmoudi [46, eqn (55)]: adapting its notation in terms of the elastic stress to $\boldsymbol{B}_e$ yields:

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho\frac{|\boldsymbol{v}|^2}{2} + \frac{G}{2\rho}\mathrm{tr}\left(\boldsymbol{B}_e - \boldsymbol{I}\right)\\ &+ \int_\Omega 2\eta_0|\boldsymbol{D}|^2\\ &\quad + \frac{G^2}{2\eta}\mathrm{tr}\left(\{(1-\alpha)\boldsymbol{B}_e^{-1} + \alpha\boldsymbol{I}\}\boldsymbol{B}_e(\boldsymbol{B}_e - \boldsymbol{I})\right) = 0\end{aligned}$$

Observe that the $\mathbf{log}\,\boldsymbol{B}_e$ term has disappeared in the free energy term, so there is no more energetic barrier for extreme strains when $\det \boldsymbol{B}_e \to 0$ i.e. when a least an eigenvalue of $\boldsymbol{h}_e$ tends to $-\infty$. Moreover, the dissipation term is also different: it could become negative for small enough $\boldsymbol{B}_e$, e.g. when $\boldsymbol{B}_e = \boldsymbol{I}/2$. This estimate is clearly suboptimal for establishing the existence of solutions. It was only recently, in 2024, that Bulíček et al. [10, eqn (1.9)] obtained, in the specific case $\alpha = 1$, an estimate which is consistent with (28). Thus, the present entropy estimate (28) for the Giesekus model, with its full range of parameter α, is new.

4.3.5. The FENE-CR *model*

Alves et al. [2, p. 153] presented in their eqns (11)-(12) a formalism that contains several possible variants of the original FENE-P model. The constitutive equations for these variants could be expressed as:

$$\begin{cases}\boldsymbol{\sigma} = -p\boldsymbol{I} + 2\eta_0\boldsymbol{D} + G\left(\dfrac{\boldsymbol{B}_e}{f(\boldsymbol{B}_e)} - \dfrac{\boldsymbol{I}}{g_1(\boldsymbol{B}_e)}\right) & \text{(29a)}\\[2ex] \eta\,\overset{\triangledown}{\boldsymbol{B}}_e + G\left(\dfrac{\boldsymbol{B}_e}{f(\boldsymbol{B}_e)} - \dfrac{\boldsymbol{I}}{g_2(\boldsymbol{B}_e)}\right) = 0 & \text{(29b)}\end{cases}$$

where the functions f and g are summarized in Table 2. Let's recap the situation, as it could be confusing. The formulation proposed by Sureshkumar et al. [69] coincides with the original FENE-P model by Bird et al. [8] with a modified elasticity parameter $\tilde{G} = (1-\beta)G$. Conversely, the formulation proposed by Housiadas and Beris [33] also coincides with the original FENE-P model with the scaling $\tilde{\boldsymbol{B}}_e = (1+\beta)\boldsymbol{B}_e$ and the change of parameters $\tilde{G} = G/(1+\beta)$ and $\tilde{\beta} = \beta/(1+\beta)$. The formulation by Housiadas and Beris [33] of the FENE-P model could be confusing here, since the state for which $\boldsymbol{\sigma}_e = \rho\psi'(\boldsymbol{h}_e) = 0$ is no more $\boldsymbol{h}_e = 0$ i.e. $\boldsymbol{B}_e = \boldsymbol{I}$. Indeed, in the YALE environment, the tensor $\boldsymbol{B}_e$ is not only a conformation tensor, that could be scaled arbitrarily, but also the reversible left Cauchy-Green tensor, and $\boldsymbol{B}_e = \boldsymbol{I}$ is expected when $\boldsymbol{\sigma}_e = 0$, assuming here that the reference configuration is a *rest state* (also called *natural state*), see e.g. Ciarlet [12, p. 90].

Finally, Chilcott and Rallison [11] proposed a distinct model, referred to as FENE-CR: this model is not reducible to the original FENE-P model. The FENE-CR model could be defined in the YATE environment by choosing the free energy ψ from (17a) unchanged from the FENE-P model and adapting the dissipation potential ϕ from (22a) by redefining the fourth-order mobility tensor $\mathbb{A}$ as

$$\mathbb{A}{:}\boldsymbol{\tau} = \mathbf{dev}\,\boldsymbol{\tau} + (1-\beta)\frac{(\mathrm{tr}\,\boldsymbol{\tau})\boldsymbol{I}}{N} \tag{30}$$

for all second order tensors $\boldsymbol{\tau}$. Note that $\boldsymbol{\tau}{:}(\mathbb{A}{:}\boldsymbol{\tau}) \geqslant (1-\beta)|\boldsymbol{\tau}|^2$ and then $\mathbb{A}$ is symmetric definite positive since $\beta \in [0, 1[$. Next, $\mathbb{A}^{-1}$ (resp. $\mathbb{A}^{\mu}$) is obtained by replacing $1-\beta$ by $(1-\beta)^{-1}$ (resp. $(1-\beta)^{\mu}$) in the expression of $\mathbb{A}$, for all $\mu \in \mathbb{R}$. Thus, ϕ is convex and the FENE-CR model also satisfies the second principle. Note that Chilcott and Rallison [11] did not use the concept of mobility introduced by Giesekus: $\mathbb{A}$ is used here as a convenience but its physical interpretation is here an open question.

Since ψ is unchanged from the FENE-P model, the elastic stress $\boldsymbol{\sigma}_e$ is still given by (18a). Obtaining the two constitutive equations is then similar to that of the Giesekus model: starting from (5a)-(5b) and expanding ψ and ϕ from (17a) and (22a), respectively, the differential constitutive

$f(\boldsymbol{B}_e)$	$g_1(\boldsymbol{B}_e)$	$g_2(\boldsymbol{B}_e)$	reference	name
$1-\frac{\beta}{N}\mathrm{tr}\,\boldsymbol{B}_e$	$1-\beta=f(\boldsymbol{I})$	$1-\beta=f(\boldsymbol{I})$	Bird et al. [8]	FENE-P
$1-\frac{\beta}{N}\mathrm{tr}\,\boldsymbol{B}_e$	$1-\beta=f(\boldsymbol{I})$	$1-\frac{\beta}{N}\mathrm{tr}\,\boldsymbol{B}_e=f(\boldsymbol{B}_e)\neq g_1(\boldsymbol{B}_e)$	Chilcott and Rallison [11]	FENE-CR
$\dfrac{1-\frac{\beta}{N}\mathrm{tr}\,\boldsymbol{B}_e}{1-\beta}$	$1=f(\boldsymbol{I})$	$1=f(\boldsymbol{I})$	Sureshkumar et al. [69]	FENE-P
$1-\frac{\beta}{N}\mathrm{tr}\,\boldsymbol{B}_e$	$1\neq f(\boldsymbol{I})$	$1\neq f(\boldsymbol{I})$	Housiadas and Beris [33]	FENE-P

Table 2: Variants of the FENE-P model where f, g_1 and g_2 functions are involved in (29a)-(29b).

equation (25a) in terms of $\boldsymbol{h}_e$ writes:

$$\overset{\circ}{\boldsymbol{h}}{}_e^{(log)} + \left(\frac{G}{2\eta}\right)\frac{\boldsymbol{I}-\mathbf{exp}(\boldsymbol{h}_e)}{1-\dfrac{\beta}{N}\mathrm{tr}\,\mathbf{exp}(2\boldsymbol{h}_e)} = \boldsymbol{D} \qquad (31)$$

after expanding $\mathbb{A}\!:\!\boldsymbol{\sigma}_e$ with (30) for the present mobility tensor $\mathbb{A}$ and (18a) for the elastic stress $\boldsymbol{\sigma}_e$. Conversely, using the kinematic relation (8b), the differential constitutive equation (26a) in terms of $\boldsymbol{B}_e$ writes:

$$\frac{\eta}{G}\overset{\triangledown}{\boldsymbol{B}}_e + \frac{\boldsymbol{B}_e-\boldsymbol{I}}{1-\dfrac{\beta}{N}\mathrm{tr}\,\boldsymbol{B}_e} = 0 \qquad (32)$$

This differential equation exactly coincides with (29b) when selecting the FENE-CR model in Table 2. Then, the reversible left Cauchy-Green tensor $\boldsymbol{B}_e$ also coincides here with the **conformation tensor**.

Also similarly to the Giesekus model, from (10) and expanding ϕ, the **dissipation** writes (see Fig. 5.right):

$$\begin{aligned}\mathscr{D} &= 2\eta_0|\boldsymbol{D}|^2 + \frac{1}{2\eta}\mathrm{tr}\,\left(\boldsymbol{\sigma}_e\left\{(\boldsymbol{B}_e^{-1}\mathbb{A})\!:\!\boldsymbol{\sigma}_e\right\}\right)\\ &= 2\eta_0|\boldsymbol{D}|^2\\ &\quad + \frac{G^2}{2\eta}\mathrm{tr}\left(\frac{\boldsymbol{I}-\boldsymbol{B}_e^{-1}}{1-\dfrac{\beta}{N}\mathrm{tr}\,\boldsymbol{B}_e}\left(\frac{\boldsymbol{B}_e}{1-\dfrac{\beta}{N}\mathrm{tr}\,\boldsymbol{B}_e} - \frac{\boldsymbol{I}}{1-\beta}\right)\right)\end{aligned}$$

after expanding $\boldsymbol{\sigma}_e$ from (18a) and (30) for the mobility tensor $\mathbb{A}$. Since $\boldsymbol{B}_e^{-1} = \mathbf{exp}(-2\boldsymbol{h}_e) > 0$ then $\boldsymbol{B}_e^{-1}\mathbb{A}$ is also a symmetric definite positive fourth-order tensor and thus $\mathscr{D} \geqslant 0$.

The **entropy estimate** follows from corollary 2 by using ψ and $\mathscr{D}$ from (17a) and the previous expression, respectively:

$$\begin{aligned}&\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho\frac{|\boldsymbol{v}|^2}{2}\\ &\qquad + \frac{G}{2}\left(\frac{N}{\beta}\log\left(\frac{1-\beta}{1-\dfrac{\beta}{N}\mathrm{tr}\,\boldsymbol{B}_e}\right) - \frac{\mathrm{tr}\,\mathbf{log}\,\boldsymbol{B}_e}{1-\beta}\right)\\ &\quad + \int_\Omega 2\eta_0|\boldsymbol{D}|^2\\ &\quad + \frac{G^2}{2\eta}\mathrm{tr}\left(\frac{\boldsymbol{I}-\boldsymbol{B}_e^{-1}}{1-\dfrac{\beta}{N}\mathrm{tr}\,\boldsymbol{B}_e}\left(\frac{\boldsymbol{B}_e}{1-\dfrac{\beta}{N}\mathrm{tr}\,\boldsymbol{B}_e} - \frac{\boldsymbol{I}}{1-\beta}\right)\right)\\ &= 0 \end{aligned} \qquad (33)$$

This entropy estimates for the FENE-CR model is new to the best knowledge of the author.

5. General discussion

The discussion begins with our relevance for reproducing known results about existing models. Then, we address the identification of the conformation tensor and the interest of its logarithm. Next, we discuss about entropy estimates in the context of proving the existence of solutions for viscoelastic fluid problems. We then turn to a preliminary exploration of the possibilities of the YATE environment for the design of new constitutive equations. Finally, we discuss the potential of diagrams for the representation of models.

5.1. Reproducing old results

Let us quote Beris and Edwards [5, p. 534], who wrote in 1990: "*In order to validate the procedures of any new formalism, it is first necessary to reproduce a few old results with the new formalism. It is quite possible that in so doing we can learn something about the character of the old results as well*".

Indeed, the second principle of thermodynamics was for the fist time successfully checked in 1990 by Beris and Edwards [5] for most common viscoelastic fluid models. With the YATE environment, we are able to prove again, in a clear and concise way, that both the Oldroyd-B, FENE-P, Giesekus and FENE-CR fluids satisfy the second principle of thermodynamics (see paragraphs 4.3.2 to 4.3.5). Instead of lengthy and complex developments, this verification bolls down here to assert the convexity of the dissipation potential ϕ: this check was trivial for all the considered models here.

The satisfaction of the second principle for the Oldroyd-B model was an open question while, in 1984, Oldroyd wrote [50, p. 43-45]:

> "*But no general analysis of the full implications of thermodynamics for the formulation of the equations of state of a flowing continuum has yet been achieved. The difficulty of generalizing thermodynamics to include irreversible phenomena is well known. The magnitude of the task of including within the scope of a generalized thermodynamics a fluid whose behavior at any time may depend on previous rheological history [...] may be appreciated when one considers what will in general be required to define the thermodynamic state of a material element. [...] The absence of [a general discussion of rheological equations of state in relation to the laws of thermodynamics] must be read as an admission of the existence of a very serious gap in present understanding of the principles governing the formulation of equations of state*".

5.2. Conformation tensor

The conformation tensor is widely used in physics as a conceptual tool for the development of new constitutive equations, in mathematics for formulating system of equations and also for numerical computations. It might seems surprising to reinterpret this tensor here as a purely kinematic one, the reversible left Cauchy-Green tensor $\boldsymbol{B}_e$. Let us therefore return to the ideas underlying the $\langle \boldsymbol{r}\boldsymbol{r}\rangle$ conformation tensor.

In 1966, Giesekus [25] wrote, in his eqn (12): $\langle \boldsymbol{r}\boldsymbol{r}\rangle = \boldsymbol{C}\,\langle \boldsymbol{r}_0\boldsymbol{r}_0\rangle$ where $\boldsymbol{C}$ denotes the dimensionless conformation tensor. From Fig. 3, the current configuration represents the space for the dumbbell vectors $\boldsymbol{r}$ while the intermediate configuration is for $\boldsymbol{r}_0$. In this paper, he just mentioned that the $\boldsymbol{C}$ tensor represents a "*spatial strain measure*" ("*rämliche deformations-maße*") and, in footnote 8 on the same page, he only indicated that it was "*occasionally referred to as the Finger strain measure*" ("*gelegentlich als Fingersches deformationsmaß*"). From the official nomenclature [17, p. 10], the $\boldsymbol{C}$ Finger tensor could either coincide with $\boldsymbol{B}_e$ or with $\boldsymbol{C}_e^{-1}$, i.e. the inverse of the reversible right Cauchy-Green tensor. Unfortunately, there was no more kinematic development in this paper and the "*Finger tensor*" terminology remains too imprecise. However, the details of the development of this tensor were contained in an earlier article by Giesekus [24] from 1962. In this earlier paper, he assumed that the reference configuration is a "*rest state*" ("*Ruhezustand*") with an isotropic configuration tensor i.e. $\langle \boldsymbol{r}_0\boldsymbol{r}_0\rangle = r_0^2\boldsymbol{I}$. In his eqn (20), he also introduced the gradient of the transformation $\boldsymbol{A}$ and its transpose $\tilde{\boldsymbol{A}}$: with current notations, $\boldsymbol{A}$ is denoted as $\boldsymbol{F}_e$. In (21), he explained that a vector $\boldsymbol{r}_0$ from the reference configuration is transformed as $\boldsymbol{r} = \boldsymbol{F}_e\boldsymbol{r}_0$. So that his eqn (22) writes with the present notations $\langle \boldsymbol{r}\boldsymbol{r}\rangle = r_0^2\boldsymbol{F}_e\boldsymbol{F}_e^T$ i.e. $\boldsymbol{B}_e = \boldsymbol{F}_e\boldsymbol{F}_e^T$ represents the Giesekus dimensionless conformation tensor.

Thus, Giesekus's choice coincides with the present result, obtained spontaneously with the YATE environment. After 1966, the concept of conformation tensor was considerably developed in the monograph by Bird et al. [7], in the context of kinetic theories, and eventually, its kinematic origins were forgotten. Giesekus wrote these two articles from 1962 and 1966 in German, so they were less read than his famous paper [26] from 1982. The paper from 1962 has been translated by the present author [64] and is freely available while Germann et al. [23] also have translated the 1966 one.

5.3. Logarithm of the conformation tensor

The concept of *logarithm of the conformation tensor* was introduced in 2004 by Fattal and Kupferman [21]: these authors were motivated by the development of robust numerical methods. Since this, in the viscoelastic fluid community, the change of variable from the conformation tensor to its logarithm is still considered as a pure numerical trick, without any physical interpretation.

From the previous identification of the left Cauchy-Green tensor $\boldsymbol{B}_e$ as the conformation tensor, it follows that the left Hencky strain $\boldsymbol{h}_e = (1/2)\,\mathbf{log}\,\boldsymbol{B}_e$ identifies, up to a half factor, to this logarithm of the conformation tensor. All the nonlinear complex and obscure terms appearing in the previous formulation in terms of the logarithm of conformation formulation are now reinterpreted as a clear and natural concept: the logarithmic corotational derivative (definition 7). In consequence, observe the hight readability and compactness of the formulation (14) of the Oldroyd-B model in terms of the reversible left Hencky strain $\boldsymbol{h}_e$. The same is true for the formulation of the FENE-P (18c), Giesekus (25b) and FENE-CR (31) models. The advantage of the formulation in $\boldsymbol{h}_e$ is not limited to its high readability.

When proving the second principle and also establishing the entropy estimate, the tensor $\boldsymbol{B}_e$ should be symmetric definite positive. When using constitutive equations formulated in terms of $\boldsymbol{B}_e$, this is not an obvious task: we must prove that it remains definite positive during all its evolution, see e.g. Hulsen [35] or Beris and Edwards [6, p. 272-281]. The situation is very different when using the formulation with $\boldsymbol{h}_e$: the tensor $\boldsymbol{B}_e = \mathbf{exp}(2\boldsymbol{h}_e)$ always remains definite positive while $\boldsymbol{h}_e$ runs through the entire range of symmetric tensors. For instance, we directly conclude from (15) that the dissipation of the Oldroyd-B model is always non-negative for any tensor $\boldsymbol{h}_e$ without any need of supplementary proof. The tensor $\boldsymbol{h}_e$ is therefore not only useful for computing numerical solutions: it offers a definite theoretical advantage over others formulations.

In 2011, Balci et al. [3] proposed an alternative for preserving the positivity of the conformation tensor by using its square root instead of its logarithm. The kinetic interpretation of the square root is the left stretch tensor $\boldsymbol{V}_e = \boldsymbol{B}_e^{\frac{1}{2}}$. Nevertheless, while $\boldsymbol{B}_e = \boldsymbol{V}_e^2$ remains positive for any $\boldsymbol{V}_e$, the left stretch tensor $\boldsymbol{V}_e$ itself also should remain definite positive during its evolution for maintaining the consistency of the mathematical formulation: due to numerical approximations, this constraint could be violated during computations and then, the approximate solution would be likely to blow up. Thus, the difficulty of maintaining the strict positivity constraint on an approximate tensor remains: it appears to be shifted from $\boldsymbol{B}_e$ to $\boldsymbol{V}_e$. Finally, experiences show that numerical resolutions in terms of $\boldsymbol{h}_e$ are significantly more robust than others.

$$\begin{tikzcd}
 & \text{enthalpy} & s : \theta \arrow[dddd, dash, dotted] & \text{Gibbs} & \\
 & \mathscr{H}(s,\boldsymbol{\sigma}) \arrow[rr, leftrightarrow] \arrow[dd, leftrightarrow] & & \mathscr{G}(\theta,\boldsymbol{\sigma}) \arrow[dd, leftrightarrow] & \\
 \begin{array}{c}\boldsymbol{\sigma}\\ \boldsymbol{h}\end{array} \arrow[rrrr, dash, dotted] & & & & \begin{array}{c}\boldsymbol{\sigma}\\ \boldsymbol{h}\end{array} \\
 & e(s,\boldsymbol{h}) \arrow[rr, leftrightarrow] & & \psi(\theta,\boldsymbol{h}) & \\
 & \text{internal} & s : \theta & \text{free} &
\end{tikzcd}$$

Figure 6: Thermodynamic energies: commutation diagram via the Legendre transformation.

The left Hencky strain $\boldsymbol{h}$ presents amazing properties. The strain $\boldsymbol{h}$ is the only strain measure such that the strain rate $\boldsymbol{D}$ expresses as a corotational derivative, see (8c). For an isotropic elastic material, the Hencky strain $\boldsymbol{h}$ is also the only strain measure such that his conjugacy stress via the free energy ψ is the elastic stress $\boldsymbol{\sigma}$, i.e. $\boldsymbol{\sigma} = \rho\partial_{\boldsymbol{h}}\psi(\boldsymbol{h})$, see [63, p. 80]. The Legendre transform of the free energy $\psi(\boldsymbol{h})$ is the Gibbs energy $\mathscr{G}(\boldsymbol{\sigma})$ and, similarly to (2e), the optimality relations write:

$$\begin{aligned}
&\rho\psi(\boldsymbol{h}) = \rho\mathscr{G}(\boldsymbol{\sigma}) + \boldsymbol{\sigma}\!:\!\boldsymbol{h} \\
&\text{with } \boldsymbol{h} = -\rho\frac{\partial\mathscr{G}}{\partial\boldsymbol{\sigma}}(\boldsymbol{\sigma}) \text{ and } \boldsymbol{\sigma} = \rho\frac{\partial\psi}{\partial\boldsymbol{h}}(\boldsymbol{h})
\end{aligned} \tag{34}$$

Combining the two commutations (2e) and (34), we obtain the commutation diagram from Fig.6, where we also introduced the enthalpy. The two conjugate pairs (s,θ) and $(\boldsymbol{h},\boldsymbol{\sigma})$ represent the fundamental thermodynamic state variables for the description of thermal and dynamic aspects, respectively. This extends to more complex materials in terms of $(\boldsymbol{h}_e,\boldsymbol{\sigma}_e)$: instead of using ψ or e, we could also use the enthalpy $\mathscr{H}$ or the Gibbs energy $\mathscr{G}$ for specifying a material.

Finally, in the context of complex fluids, we have found that the reversible left Hencky strain $\boldsymbol{h}_e$ is the most appropriate variable for both theoretical considerations and practical numerical computations. It represents the cornerstone of the YATE environment. It could become a new starting point for establishing proofs of the existence of solutions. In the next section, we review the available existence results and study how the YALE environment could contribute.

5.4. Entropy estimate and existence results

In the introduction, we reviewed how, in 2007, Hu and Lelièvre [34, p. 914] established an **entropy estimate** for both the Oldroyd-B and the FENE-P models. Soon, in 2011, based on this major result, Masmoudi [46] showed for the first time a global **existence result** for both the FENE-P and Giesekus models.

The YATE environment furnishes a new method to directly establish entropy estimates for a general class of continuum models, thanks to corollary 2. We re-obtain the two important entropy estimates shown in 2011 by Hu and Lelièvre [34] for Oldroyd-B and FENE-P models: see (16) and (21). Moreover, we also provide in this paper two new entropy estimates for the Giesekus and FENE-CR models: see (28) and (33).

For the FENE-P model, Masmoudi [46] used the entropy estimate provided by Hu and Lelièvre [34]. In the same paper, Masmoudi [46] addressed also the Giesekus model and since no *a priori* bounds was available for this model, he proposed his own. From the discussion at the end of paragraph 4.3.4, his proposition appears to be less efficient than the present entropy estimate (28), based on thermodynamics. Only recently, in 2024, Bulíček et al. [10] established an entropy estimate for a special case of the Giesekus model which is compatible with the present one. They also proved a stronger global-in-time existence result. Finally, these repeated experiences show that thermodynamics provides entropy estimates which lead to very efficient *a priori* bounds for proving existence results.

Based on current knowledge, the FENE-P and Giesekus models offers better guarantees of well-posedness than the Oldroyd-B one. Therefore, these two models are very attractive, both from a physical and mathematical point of view.

In the next section, we turn to a preliminary exploration of the YATE environment for the design of new models.

5.5. Exploration toward new models

Fig. 7 presents an overview of some possibilities provided by this new environment. Each table lists in the left and right columns the most common free energies ψ and dissipation potentials ϕ. And, as a lego game, we explore some possible combinations. Fig. 7.top-left shows that, by combining a zero free energy with a quadratic dissipation potential, we obtain a Newtonian fluid. Replacing the dissipation by a Bingham or an Herschel-Bulkley one, we obtain the corresponding viscoplastic fluid. Fig. 7.top-center turns to the neo-Hookean free energy ψ. Combining with a zero dissipation potential, we get the neo-Hookean elastic solid, as proposed by Blatz [9]. Turning to a quadratic dissipation potential, the Oldroyd-B viscoelastic fluid is obtained. Changing to the dissipation potential proposed by Giesekus [26] (see paragraph 4.3.4), we obtain the corresponding model. Choosing a Bingham or Herschel-Bulkley dissipation potential, the corresponding elastoviscoplastic fluid [59, 60] is obtained. Fig. 7.top-right explores some combinations with the FENE-P free energy ψ. Combining with a zero dissipation potential, we get a FENE-P elastic solid, as proposed by Gent [22]. Choosing a quadratic dissipation potential, the original FENE-P viscoelastic fluid proposed by Bird et al. [8] is obtained. Note that the elastic solid version was developed later by Gent [22], in 1996, independently of its viscoelastic fluid version, proposed in 1980 by Bird et al. [8]. Next, combining with the Giesekus dissipation potential (see paragraph 4.3.4), we obtain the hybrid FENE-P-Giesekus viscoelastic fluid due to Stephanou et al. [68]. Finally, combining with a Bingham or Herschel-Bulkley dissipation potential, we obtain an hybrid FENE-P-elastoviscoplastic fluid, see Izbassarov et al. [39] for a similar idea, without a thermodynamic setting, however.

It is also possible to develop a new free energy ψ, or to reuse one of the many formulas that have been developed for elastic solids in large-strains. Fig. 7.center-right shows how to combine it with all existing dissipation potentials. Conversely, Fig. 7.bottom proposes developing new dissipation potential and combining it with old or new free energy.

Indeed, one of the strengths of the YATE environment is to offer a unified presentation of fluids and solids, see also Snoeijer et al. [67] for a discussion on this type of unification. Let us point out that, for all the new models designed from this environment, an entropy estimate will immediately be available thanks to corollary 2. Thus, the proof of existence of solutions could start now without any retard.

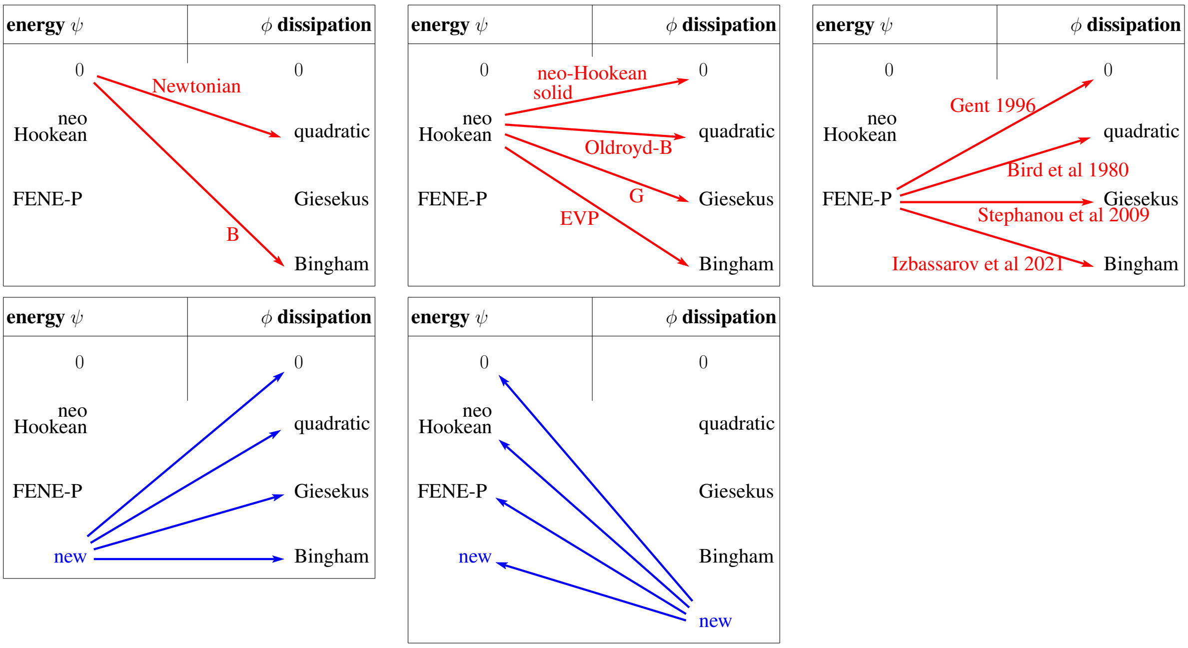

Figure 7: Exploration of the thermodynamic environment: combining old and new free energy ψ and dissipation potential ϕ.

Finally, let us quote Beris and Edwards [5, p. 534] again, who wrote in 1990: "*As a final comment, let us state that the generalized bracket formulation outlined above will not (and was not intended to) supplant either traditional continuum mechanical modeling procedures or kinetic theory developments. The idea was to show that an additional method of formulation exists, which may become useful when traditional techniques are inadequate or too complicated to apply successfully*". Indeed, the development of a new model generally bases on experimental observations, often supplemented by microstructural hypotheses and optionally with the help of kinetic theories. Although compliance with the second principle is necessary to avoid any unphysical predictions, it is not sufficient. Thanks to the proposed methodology, the thermodynamic aspect could now be more easily integrated from the earliest stages of continuous modeling.

5.6. *Diagrams*

The present extension to large-strain in an Eulerian frame of the standard generalized material conserves its original clear and easy-to-use interface. Indeed, starting from a rheological diagram, as on Fig. 4, we are able to specify both the free energy ψ and the dissipation potential ϕ.

We have just to collect in ψ all the elements of the diagram that are associated to reversible processes (e.g. springs) while, all the others elements, which are associated to irreversible processes (e.g. dashpots, breaks) go in ϕ.

Then, constitutive equations are automatically obtained from (9a)-(9b) by simple differentiations. The second principle is easy to check: the convexity of ϕ is sufficient. Also, the dissipation potential ϕ could be non-smooth, as for the Bingham fluid model: so this environment supports applications in plasticity, damage and friction.

Let us mention that some models require to split the strain in more than two parts. For instance, the Isayev and Fan [37] elastoviscoplastic model represented in Fig. 8 splits the strain as $\boldsymbol{h} = \boldsymbol{h}_e + \boldsymbol{h}_{pe} + \boldsymbol{h}_{pp}$. This split could be obtain by introducing two intermediate configurations, the first one as $\boldsymbol{\chi} = \boldsymbol{\chi}_e \circ \boldsymbol{\chi}_p$ and the second one with $\boldsymbol{\chi}_p = \boldsymbol{\chi}_{pe} \circ \boldsymbol{\chi}_{pp}$ such that $\boldsymbol{\chi} = \boldsymbol{\chi}_e \circ \boldsymbol{\chi}_{pe} \circ \boldsymbol{\chi}_{pp}$. This operation could be applied recursively, such that the strain splits in an arbitrarily number of parts $\boldsymbol{h} = \sum_i \boldsymbol{h}_i$.

Non-trivial but isotropic tensor constitutive equations can always be decomposed into deviatoric and trace parts, and the two corresponding dia-

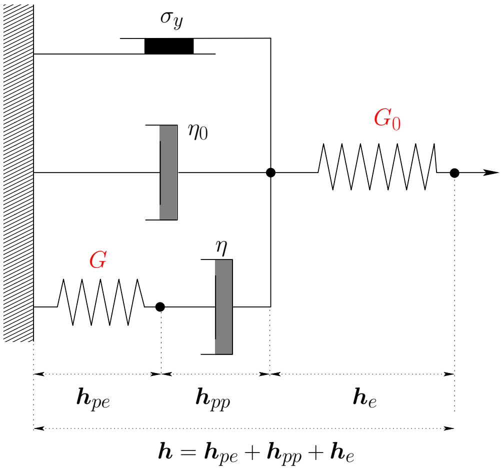

Figure 8: Recursive split of the strain for the Isayev and Fan [37] model.

grams can be represented. Nevertheless, both the Oldroyd-B, FENE-P, Giesekus and FENE-CR models share the same diagram, see Fig. 4. Indeed, the nonlinear subtleties that differentiate these models is not represented. Diagrams therefore provide a visual guide to the main kinematic and thermodynamic structure of the model, but the fine details remain in the mathematical expressions of ψ and ϕ.

6. Conclusion

Until now, the development of a new fluid model began in most cases with the direct writing of the constitutive equations. Then, often long time later, we moved on to verifying the second principle of thermodynamics: the proof could take a long time. Later still, we began working on entropy estimates and existence results. For instance, the Oldroyd-B model was developed in 1950, and it took about 50 years to prove that it satisfied the second principle and a further 21 years to obtain its entropy estimate. Furthermore, the existence of solutions for this model remains an open problem, although work on this began more than 30 years ago.

The present paper provides a **new method** to automatically obtain **entropy estimates** together with an explicit expression for the dissipation. This approach is demonstrated for both the Oldroyd-B, FENE-P, Giesekus and FENE-CR models. And these estimates was obtained after only few lines of computation. While these estimated have already been obtained with difficulties and backtracking for the Oldroyd-B and FENE-P models, these estimates are here new for the Giesekus and FENE-CR models.

The **conformation tensor** has been identified in terms of the reversible Cauchy-Green tensor $\boldsymbol{B}_e$. Consequently, the formulation in terms of the logarithm of conformation tensor has been reinterpreted in terms of the Hencky strain $\boldsymbol{h}_e$ and its **logarithmic corotational derivative**: although useful for numerical calculations, this also leads to much more concise and understandable formulations, but above all, it opens up new avenues for theoretical developments.

Based on a **unified presentation of fluids and solids**, we propose a **new methodology** for macroscopic continuum modeling: we suggest that the model designers specify the free energy ψ and the dissipation potential ϕ from the earliest stages of developing a new continuous model. It is then easy to check whether the second principle of thermodynamics is satisfied: in most cases, the convexity of ϕ is sufficient. Next, the constitutive equations are obtained automatically by a simple derivation of ψ and ϕ. In addition, an entropy estimate (*a priori* bound) is also directly obtained without effort. Using this methodology, we guarantee that future mathematical models will not risk predicting something like the ball of Fig. 1 bouncing higher and higher.

Future work will, of course, focus first on studying others existing models: we will examine their thermodynamic properties and provide their entropy estimate. In a preliminary exploration, we showed how this clear and efficient environment could be used to develop new models: this effort will be continued. Applications to granular materials, with strongly nonlinear and non-smooth potentials will be considered, e.g. extending to large-strains the model presented in [62]. Also, the development of models for active materials and biological tissues, involving polarity and micro-rotations, is a challenging task for continuum modeling.

Appendix A. Proof of the global estimates

This appendix contains the proofs of theorem 1 and corollary 2.

Let us multiply (2b) by $\boldsymbol{v}$, add (2c) and sum over Ω:

$$\int_\Omega \rho \, \overset{\bullet}{\overbrace{\left(\frac{|\boldsymbol{v}|^2}{2}+e\right)}} = \int_\Omega \operatorname{div}\left(\boldsymbol{\sigma v}+\boldsymbol{q}\right)+\boldsymbol{f}.\boldsymbol{v}+r \tag{A.1}$$

Note that, for any function φ, the Reynolds formula leads to

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho\varphi &= \int_\Omega \partial_t(\rho\varphi)+\operatorname{div}(\rho\varphi\boldsymbol{v}) \\ &= \int_\Omega \rho\dot{\varphi}+\left(\dot{\rho}+\rho\operatorname{div}\boldsymbol{v}\right)\varphi \\ &= \int_\Omega \rho\dot{\varphi} \end{aligned} \tag{A.2}$$

after using the mass conservation (2a). Applying (A.2) with $\varphi = (1/2)|\boldsymbol{v}|^2+e$ to (A.1) and using the divergence formula on the right-hand-side yields

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho\left(\frac{|\boldsymbol{v}|^2}{2}+e\right) &= \int_\Omega \boldsymbol{f}.\boldsymbol{v}+r+\int_{\partial\Omega}(\boldsymbol{\sigma n}).\boldsymbol{v}-\boldsymbol{q}.\boldsymbol{n} \\ &= 0\end{aligned}$$

since the system is isolated, see definition 1. Then (3a) is established.

The growing global entropy formula (3b) is obtain by a sum over Ω of (2d) and applying (A.2) with $\varphi = s$. Then, the proof theorem 1 is complete.

Let us turn now to the isothermal estimate of corollary 2. From (3a) and expanding $e = \psi + s\theta$ from (2e), we get

$$\begin{aligned}\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho\left(\frac{|\boldsymbol{v}|^2}{2}+\psi\right) &= -\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho s\theta \\ &= -\theta\frac{\mathrm{d}}{\mathrm{d}t}\int_\Omega \rho s \\ &= -\int_\Omega \mathscr{D}\end{aligned}$$

since θ is constant and using (3b). Then (4) is established and the proof corollary 2 is complete.

Appendix B. Relation with the Poisson bracket formalism

This appendix provides the correspondence, for viscoelastic fluid models, between the present notations and the Poisson bracket formalism developed in 1990 by Beris and Edwards [5] (see also [6, chap. 8]). The reversible left Cauchy-Green tensor $\boldsymbol{B}_e$ coincides with the dimensionless conformation tensor while a dimensional conformation tensor $\boldsymbol{c} = (k_B T/K)\,\boldsymbol{B}_e$ is used in the Poisson bracket formalism. Here K is the elastic Hookean spring constant, T is the temperature and k_B is the Boltzmann constant. The elastic modulus $G = nk_BT$, where n is the number density of elastic connectors. This formalism bases on the concept of Hamiltonian H. For a viscoelastic fluid, the Hamiltonian splits as $H(\boldsymbol{v},\boldsymbol{c}) = K(\boldsymbol{v}) + A(\boldsymbol{c})$ where A is related to the free energy ψ as $A(\boldsymbol{c}) = \int_\Omega \rho\psi$. The elastic stress writes $\boldsymbol{\sigma}_e = \rho\psi'(\boldsymbol{h}_e) = 2\boldsymbol{c}\,A'(\boldsymbol{c})$. The dissipation potential ϕ was not introduced in the bracket formalism: it uses the Onsager matrix concept instead. Since variables are second-order tensors, this matrix with non-constant coefficients is represented by a fourth-order tensor function $\mathbb{A}(\boldsymbol{c})$. The second principle is then classically checked via the non-negativity of $\mathbb{A}(\boldsymbol{c})$. Despite the dissipation $\mathscr{D}$ was not provided explicitly in closed form in these publications, it could be computed from $\int_\Omega \mathscr{D} = [H,H]$ where the notation $[.,.]$ is referred to as the square bracket. For instance, for the incompressible upper-convected Maxwell viscoelastic fluid, i.e. the Oldroyd-B model from section 4.3.2 when the solvent viscosity $\eta_0 = 0$, the free energy is $A(\boldsymbol{c}) = \int_\Omega (n/2)(K \operatorname{tr}\boldsymbol{c} - k_B T \log\det\boldsymbol{c})$, the dissipation tensor is $\mathbb{A}(\boldsymbol{c}) = (8/(n\zeta))\,\boldsymbol{c}$ where $\zeta = 4\eta K/G$ is the drag coefficient, and, expanding $[H,H] = A'(\boldsymbol{c})\!:\!\mathbb{A}(\boldsymbol{c})\!:\!A'(\boldsymbol{c})$, we fall back to (15).

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